MERCK

MYCS 2025

BOOK OF ABSTRACT

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INSTM

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Welcome to the 24th edition of the Merck Young Chemists' Symposium (MYCS), formerly also known as SAYCS and MEYCS. This international conference is organized by the Young Group of Società Chimica Italiana (SCI Giovani) and the National Interuniversity Consortium of Materials Science and Technology (INSTM) with the financial support from Merck and several other sponsors, that you will meet during the conference.

The symposium covers all the disciplines of Chemistry, aiming to connect young researchers, inspire new ideas, and potentially trigger new collaborations. With the contributions of our five invited plenary speakers, and the international environment guaranteed by the presence of people coming from different countries, we truly hope that you will all enjoy this great event with us. We have worked hard to organize this meeting with 226 participants, prioritizing high-level scientific topics and other themes of crucial importance in our modern society. Thank you for the great trust shown towards SCI Giovani, Merck and all our supporters. Enjoy the conference and have a nice stay with us!

Signature

Marco Mendolicchio
SCI Giovani Coordinator

MYCS 2025

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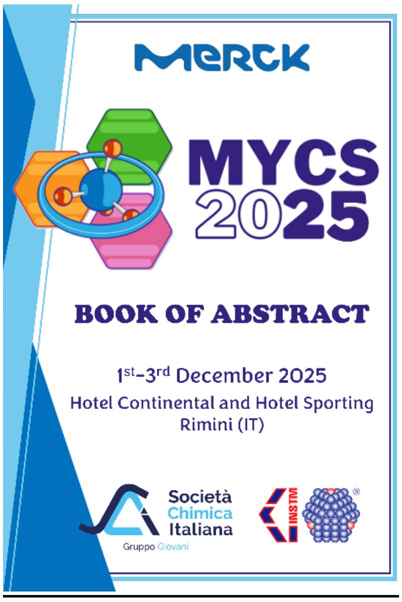MERCK MYCS 2025 BOOK OF ABSTRACT 1st-3rd December 2025 Hotel Continental and Hotel Sporting Rimini (IT) Società Chimica Italiana Gruppo Giovani INSTM	All the scientific contributions of the symposium are collected in this international volume with ISBN code. You can cite your work as follows: N. Surname, N. Surname, g and N. Surname, <Abstract title>, in Proceedings of the Merck Young Chemist's Symposium 2025, XXIV Ed. L. Alessandroni, M. Bonomo, C. Brondi, A. Cappitti, A. Cerrato, M. Da Pian, A. Dall'Anese, D. Del Giudice, G. Falcone, A. C. Maccari, Marotta, F. Massabò, A. Massaro, M. Mendolicchio, M. Miciaccia, E. Palazzi, L. Paterlini, F. Pizzetti, L. Riva, A. Romero, E. Rossi. ISBN: 978-88-94952-58-2, 225, 2025, Rome.

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PL01

Communicating Chemistry on Social Media

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Is There a Better Way to Talk About Science? Communicating science effectively remains a complex challenge. While there is no single definitive answer, certain naive and counterproductive approaches can (and should) be avoided. This presentation explores strategies for communicating chemistry in the digital age, with a focus on social media dynamics. Key topics include the spread of fake news, scientific misinformation, public distrust, and the role of denialism and pseudoscience. Through contextual analysis, the session aims to dismantle common misconceptions and offer constructive pathways toward more effective science communication.

PL02

A microwave route to recover strategic metals from spent battery

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The growing demand for critical raw materials driven by the transition to electric mobility and renewable energy has exposed the vulnerability of current supply chains, especially for lithium-ion batteries (LIBs). In response, the CARAMEL project introduces an innovative, sustainable solution based on a newly patented technology for the recovery of strategic metals from spent LIBs [1]. Unlike traditional pyrometallurgical and hydrometallurgical approaches—which are energy-intensive and chemically aggressive—this method enables selective, low-impact extraction of high-value materials using a microwave-assisted carbothermic process [2]. The technology allows for the efficient recovery of lithium, cobalt, and manganese and supports the reuse of the obtained materials [3].

By minimizing waste and enabling direct reuse of recovered compounds, this approach embodies the principles of the circular economy. The development of a dedicated pilot plant further supports the industrial scalability of the process, offering a viable route to reduce raw material dependency and environmental footprint while enhancing resource security and economic resilience in the EU battery sector.

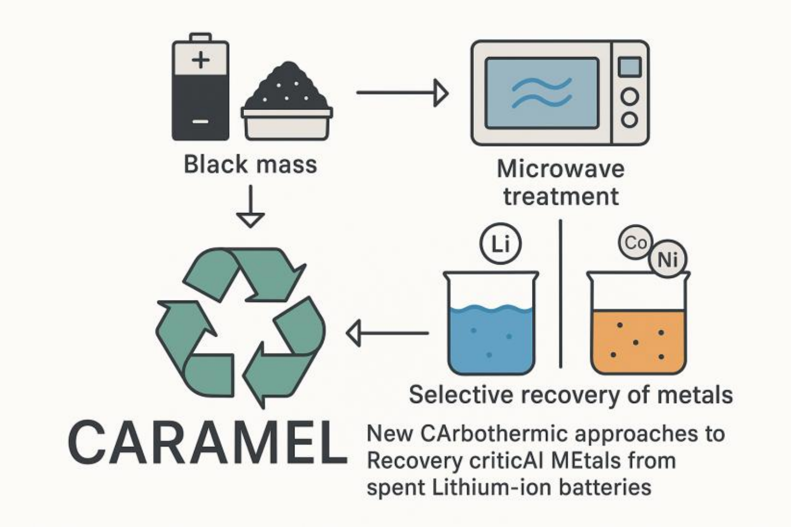

Figure 1: Scheme of the CARAMEL project.

[1] https://caramel.unibs.it/.
[1] A. Cornelio, et al., Recovery of NMC-lithium battery black mass by microwave heating processes, Energy Storage Materials, 72 (2024) 103703.
[3] A. Zanoletti, et al., AI-driven identification of a novel malate structure from recycled lithium-ion batteries, Environmental Research, 267 (2024).

PL03

From cyclodextrins to porous organic frameworks: my journey during the last twenty years

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The aim of the lecture is the one to look back at the main moments of my academic career. Going from the study of host-guest complexes formed by cyclodextrins,[1] to catalytic and sensing ability of porous organic polymers, through the use non-conventional solvents, like ionic liquids and deep eutectic solvents,[2] I have had the possibility to conjugate my interest in Supramolecular Chemistry with the one in Green Chemistry.[3]

I will try to describe the reasons that, during the years, pushed me to change directions of my research activity, problems and opportunities that characterized different steps on my way.

All aspects will be discussed also in the light of my teaching activity and membership to the life of scientific societies.

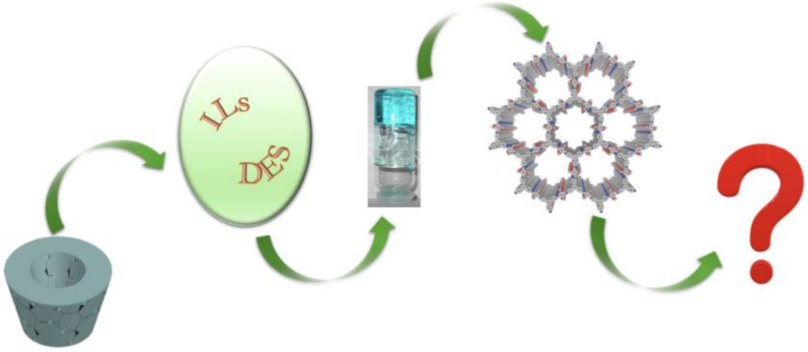

Figure 1: The steps of the research activity

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[1] F. D'Anna, S. Riela, P. Lo Meo, M. Gruttadauria, R. Noto *Tetrahedron: Asymmetry* 13 (2002) 1755-1760.
[2] S. Marullo, A. Meli, F. D'Anna *ACS Sustainable Chem. Eng.* 8 (2020) 4889-4899.
[3] S. Marullo, F. Petta, G. Infurna, N. T. Dintcheva, F. D'Anna *Green Chem.* 25 (2023) 4513-4527.

PL04

Perovskite-inspired materials: powering the next-generation of indoor photovoltaics

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The demand for energy-autonomous Internet-of-Things (IoT) devices is rapidly increasing, with billions of wireless sensors expected to be deployed in the coming decade. Indoor photovoltaics (IPVs) offer a promising solution by utilizing the abundant indoor light available in buildings. Recently, solution-processed absorbers like lead halide perovskites (LHP) have shown significant potential for efficient indoor light harvesting. However, the toxicity and bioavailability of lead is a showstopper for the widespread commercialization of LHP-based IPVs, especially given the proximity of these devices to end users in indoor environments.

Perovskite-inspired materials (PIMs) comprising Group VA pnictogen cations, such as antimony (III) (Sb3+) and bismuth (III) (Bi3+), have emerged as eco-friendly and air-stable alternatives [1]. Notably, two-dimensional PIMs such as $Ag_3Sb_2X_9$ and Cs_2AgBi2I9 exhibit quasi-direct bandgaps that are well-suited for photovoltaic and other optoelectronic applications. Despite their potential, PIMs often form disordered structures with numerous surface defects, vacancies, and grain boundaries, which limit their performance as photovoltaic absorbers. Their nearly ideal bandgap for indoor light harvesting, combined with exceptional air stability and low toxicity, inspired us to enhance their intrinsic defect tolerance through comprehensive composition engineering at each crystallographic site (A, B, X) of the PIM structure. This strategy led to a significant improvement in the performance and operational stability of pnictogen-based devices for sustainable indoor light harvesting [2,3].

[1] G. K. Grandhi, D. Hardy, M. Krishnaiah, B. Vargas, B. Al-Anesi, M.P. Suryawanshi, D. Solis-Ibarra, F. Gao, R.L.Z. Hoye, and P. Vivo, *Adv. Funct. Mater.* 34 (2024) 2307441.

[2] N. Lamminen, J. Karlsson, R. Kumar, N. S. M. Viswanath, S. Lal, F. Fasulo, M. Righetto, M. Krishnaiah, K. Lahtonen, A. Tewari, A. Katerski, J. Lahtinen, I. Oja Acik, E. M. J. Johansson, A. B. Muñoz-García, M. Pavone, L. M. Herz, G. K. Grandhi, and P. Vivo, *EES Solar* 1 (2025) 139-156.

[3] N. Lamminen, J. Lahtinen, M. Krishnaiah, J. Karlsson, M. Saju, G. K. Grandhi, and P. Vivo, *ACS Energy Lett.* 10 (2025) 3415-3418.

PL05

Venturing in Research & Innovation: How they are changing to adapt onto new challenges

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Following IInd World War, Italian and continental academia were based on a German elitist model; the aim was to create a governing class of few high-skilled citizens. In recent years, due to political changes, incremental consumes and growing population the model was not suited anymore to serve the purpose. Therefore, it has been adapted through a few reforms. At the European Union level this was also mirrored by many reforming changes at policy level on how research and innovation grants were released, the last one seeing the compulsory participation of industry together with academia into grant-schemes. So one question arises: How we are adapting to these changes? Are we still leading the pack in higher education? Is Eu still competitive in research and Innovation? How different model (e.g. Asia) are doing?

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OR89 – Sara Rossi (UniParma)

OR01

Theoretical investigation of the OH-initiated atmospheric degradation mechanism of fluorinated ethers

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The identification of chlorofluorocarbons (CFCs) as potent ozone-depleting substances prompted the urgent search for environmentally safer alternatives. Hydrofluorocarbons (HFCs) and perfluorocarbons (PFCs) have been considered as substitutes because of their zero-ozone depletion potential. These compounds, however, contribute significantly to global warming. Hydrofluoroethers (HFEs), currently employed in diverse industrial applications as foam-blowing agents, refrigerants, and solvents, have emerged as promising third-generation alternatives. Their environmental advantage arises from their chemical structure (R'–O–R), which undergoes rapid atmospheric degradation. Specifically, hydrogen abstraction by hydroxyl (OH) radicals initiates the formation of alkyl radicals (R'–O–R•), while the ether linkage enhances reactivity, accelerating decomposition [1].

To gain deeper insight into the atmospheric removal processes of HFEs, we conducted a comprehensive theoretical investigation of the OH-initiated oxidation mechanisms of three fluorinated dimethyl ethers: CH_3OCF_3 (HFE-143a), CH_3OCHF_2 (HFE-152a), and CH_3OCH_2F (HFE-161). Potential energy surfaces (PESs) were characterized by optimizing geometries and computing zero-point vibrational energies at various levels of density functional theory, while electronic energies were refined using the “jun-cheap” composite scheme (jChS) [2]. Kinetic parameters were derived employing canonical variational transition state theory (CVTST) [3], with the inclusion of tunneling effects. The resulting temperature and pressure-dependent rate coefficients demonstrated excellent agreement with available experimental data, providing robust validation of the proposed mechanisms and allowing extension of rate coefficients down to temperatures of atmospheric relevance.

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[3] J. L. Bao, D. G. Truhlar, Chem. Soc. Rev. 46 (2017) 7548-7596.

OR02

Machine learning interatomic potentials for lithium thiophosphates electrolytes

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One of the most promising alternatives to Li-ion liquid technology are all-solid state batteries (ASSB), which have several advantages [1], such as greater stability, better safety, and higher energy density. But they also have an intrinsic, and still unsolved, problem caused by their solid nature, the low ion mobility. Glassy-ceramic Lithium thiophosphates, LPS (xLi_2S-$(1-x)P_2S_5$) are among the most promising electrolytes materials, and by tuning their composition is possible to optimize their performance and achieve high ion conductivities, at least 10^{-3} S/cm to be competitive with liquid electrolytes; but this is an extremely complicated task because we do not yet know deeply the structure-properties relationship; as result the optimization process requires laborious trial-and-error laboratory procedures. We can help make this process much quicker by using molecular modelling. Typically, computational approaches to electrochemistry involve ab-initio molecular dynamics (AIMD) methods, which despite their accuracy, are very slow and computationally intensive, compared to classical molecular dynamics (MD), which instead relies on parametric force fields (FF). Classical MD calculations on LPS are, at the moment, difficult to perform because they require the development of a suitable FF whose analytical form is complicated because of the different states of chemical coordination that Li+ assumes in the amorphous solid. Nevertheless, it is important for the electrochemical community to have access to a quick and efficient way to model electrolytes such as LPS.

To leverage the advantages of both methods we used deep learning molecular dynamics [2] and generated a new deep learning force field (DLFF). The deep neural network has been trained using our ab-initio data, this way the DLFF has the high accuracy [3] of the ab-initio level chosen for the training set and, being parametric, a high efficiency (classical MD level). Using this DLFF, we have performed fast and accurate simulations on model systems beyond the actual limits of AIMD in size and time scales. This way we determined the electrochemical properties of different compositions of LPS in a quick and accurate way, which was rarely achieved before. This approach will be crucial to determine electrochemical properties of LPS oxides (LPSO) and optimize their composition as well, making this technology competitive in a large-scale industrial environment.

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OR03

A thermodynamical and structural study of dimethomorph–β-cyclodextrin host–guest complexes

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Dimethomorph (DMM) is a fungicide that is widely used in agriculture and is characterised by its low solubility and moderate toxicity to aquatic organisms [1]. Thanks to its hydrophobicity, it is expected to interact well with the hydrophobic internal cavity of β-cyclodextrins (β-CDs). Due to their amphiphilic properties, these cyclic oligosaccharides are widely used to form inclusion complexes with a variety of molecules, such as pharmaceuticals and environmental contaminants [2]. In this study we investigate the binding behavior of the two isomers of dimethomorph and β-cyclodextrin. A double theoretical and experimental approach was employed to elucidate the dynamics, energetics and structural features of the host-guest complex formation. At room temperature, few transition between bound and unbound state are observed. This does not allow the estimation of the binding equilibrium constant. Therefore, molecular dynamics simulations at higher temperature were performed in order to estimate the thermodynamic parameters of the binding. Interestingly, the MD simulations showed that the cyclodextrin cavity selectively accommodates the two DMM isomers with distinct interaction patterns: the Z isomer forms a single stable complex, while the E isomer allows two of the three rings to interact with the cavity of the β-cyclodextrin (Figure 1). These findings highlight a reversible and stable inclusion mechanism, suggesting that β-CD-based systems could be promising materials for the removal of pollutants from the environment [2].

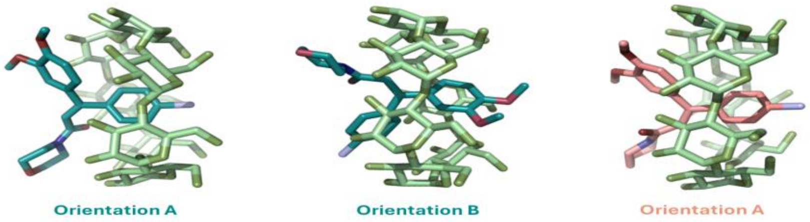

Figure 1: β-CD/DMM host-guest complexes: β-CD/DMME (green), β-CD/DMMZ (orange).

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OR04

New Insights on Hemocyanin Oxygen Transport Features: A QM/MM-NEVPT2 Perspective

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Copper-bimetallic enzymes, such as hemocyanin (Hc), play pivotal roles in oxygen transport, catalysis, and oxidative chemistry. [1-6] However, modeling these processes remains challenging due to the multireference character of the Cu_2O_2 core and its geometric flexibility, which can involve multiple isomeric forms, such as peroxo and bis-μ-oxo configurations. [7-11], influencing Hc response to oxidative stress and reactive oxygen species. In this study, we employ state-of-the-art QM/MM approaches at the NEVPT2 level (QM[NEVPT2]/MM) to investigate the Hc oxygen-binding mechanism and the peroxo-to-bis-μ-oxo isomerization. While Density Functional Theory (DFT) successfully predicts oxygen binding, it struggles to accurately describe highly correlated electronic states, such as superoxide species and mixed Cu_2 oxidation states. In contrast, NEVPT2 effectively captures these electronic complexities by accounting for both static and dynamic correlation effects. By integrating NEVPT2 within a QM/MM framework, we account for both the electronic complexity and the influence of the protein environment at feasible computational costs. Concerning the oxygen binding, our results reveal that the first electron transfer (ET) step occurs prior to the ISC, resulting in the formation of a stable singlet superoxide intermediate through a low-energy barrier. The second ET leads to the formation of a singlet oxy-Hc species featuring the characteristic peroxo-Cu_2O_2 "butterfly" core. Moreover, QM[NEVPT2]/MM predicts a lower energy barrier for the peroxo-to-bis-μ-oxo isomerization than DFT, although the peroxo form remains energetically favored within the protein environment. Overall, our findings highlight the critical roles of both the protein environment and subtle electronic correlation in accurately describing copper-oxygen interactions in complex metallo-enzymes.

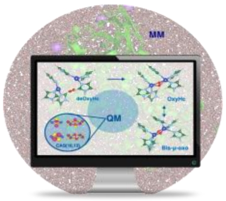

Figure 1: Scheme of QM[NEVPT2]/MM approach to unveil oxygen binding and peroxo-to-bis-μ-oxo isomerization in Hc.

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OR05

Modeling dynamic electrochemical impedance spectroscopy for hydrogen evolution reaction on single-atom catalysts

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Single-Atom Catalysts (SACs) are an emerging frontier in heterogeneous electrocatalysis. They are made of metal atoms atomically dispersed on a matrix. Computational and theoretical chemistry allow us to study catalytic processes with atomic detail and to rationalize reaction mechanisms. A lot of attention has been dedicated to the study of Hydrogen Evolution Reaction (HER) mechanism, due to its relevance in energy conversion technologies, both with computational and experimental methods. HER typically follows the Volmer-Heyrovsky-Tafel pathway: the Volmer step involves hydrogen adsorption, followed by either an electrochemical (Heyrovsky) or chemical (Tafel) desorption [1]. It has been computationally demonstrated that hydrogen complexes can form on SACs due to their analogy with homogeneous catalysts [2]. Unfortunately, it is hard to "visualize" these species experimentally. A recently developed experimental technique, dynamic Electrochemical Impedance Spectroscopy (dEIS) could be the most promising approach to study electrocatalytic reaction mechanisms [3]. In this work, we present microkinetic and dynamic Electrochemical Impedance Spectroscopy models for HER on SACs, describing Volmer-Heyrovsky and an unconventional Volmer–Heyrovsky mechanism mediated by the formation of hydrogen complexes. Our models demonstrate that simulated Tafel plots cannot always help in the visualization of hydrogen complexes formation unlike simulated electrochemical impedance spectra. This study highlights the potential of combining advanced electrochemical techniques with theoretical modeling to unravel electrocatalytic mechanisms at the atomic scale, contributing to the rational design of next-generation catalysts for sustainable energy applications.

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OR06

Spectroscopic analyses of H2O:CO2 ices in simulated space environments: a preliminary study in support of the JUICE Mission

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JUpiter ICy moons Explorer (JUICE) is a space mission that aims to make detailed observations (with a suite of remote sensing, geophysical and in situ instruments) of the planet Jupiter and its satellites Ganymede, Callisto and Europa, also known as Galilean moons. The mission's purpose is to study the Jupiter system as an archetype for gas giant planets across the Universe, explore Jupiter's complex environment in depth, and characterise its satellites (as both planetary objects and potential habitats). Our knowledge of the chemical and physical properties of solar system planets and their satellites is also based on the comparison between astronomical observations and laboratory data. As an example, infrared spectra of the surface of planetary objects obtained through astronomical observations are compared to infrared spectra of laboratory samples in order to infer the chemical composition of planetary surfaces. In addition, during the evaluation of spectroscopy data, it is essential to consider that the surfaces of planetary bodies without an atmosphere are continuously bombarded by energetic particles (such as solar wind, solar energetic particles, and magnetospheric ions) and undergo thermal cycles during their orbital motion. In this landscape, in preparation for the study of spectroscopic data from the JUICE mission, we conducted preliminary laboratory experiments aimed to simulate the icy surfaces of the Galilean satellites. Specifically, H_2O:CO_2 ices mixtures with different ratios were layered on infrared-transparent substrates in ultra-high vacuum conditions and at very low temperatures (15-300 K) [1]. The samples were characterized by FT-IR transmission spectroscopy in the 5000-500 cm^{-1} range. This spectral range includes the spectral coverage of the MAJIS (Moons And Jupiter Imaging Spectrometer) instrument onboard JUICE [2]. Here we present some preliminary experimental results relative to icy samples that suffered thermal cycles and ion irradiation (200 keV). The results represent a first step toward building a spectral reference database to support the interpretation of JUICE observations of Jupiter's icy moons. The Italian participation to JUICE mission is founded by the Italian Space Agency (ASI). This work has been developed under the ASI-INAF agreement n. 2023-6-HH.0

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OR07

Life cycle assessment of an inulin-loaded biodegradable poly(butylene adipate-co-terephtalate) (PBAT) composite material for packaging and agricultural applications

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In recent times, concerns associated with the growing consumption of fossil resources and pollution issues related to the presence of plastics in ecosystems led to a growing interest in the production of bio-based and biodegradable polymeric products. Under these circumstances, poly(butylene adipate-co-terephtalate) (PBAT) was identified as a potential biodegradable alternative to conventional materials used for packaging such as low-density polyethylene; the integration of the polymer with a natural renewable filler, e.g. inulin, could improve the mechanical properties of the material while reducing its dependance on fossil resources. To evaluate the environmental profile of the innovative material, its life cycle impacts must be calculated. In this study, a cradle-to-gate life cycle assessment (LCA) was conducted to identify the hotspots associated with the manufacture of 1 kg of a composite with a 95:5 PBAT:Inulin formulation; i.e., the fossil-based production of commercial PBAT, the production of inulin and the integration processes (such as PBAT milling and composite extrusion) were evaluated. Further sensitivity analyses were conducted to estimate how impacts differed when using bio-based PBAT to replace its fossil alternative. The investigation was conducted using the ReCiPe 2016 method, allowing to evaluate impacts across 18 midpoint and 3 endpoint categories, and the IPCC 2021 method, focusing on the carbon footprint of the product. Results showed that fossil PBAT production entailed most of the overall burdens of the composite (74% of the composite carbon footprint), followed by the consumption of electricity to conduct the integration of the polymer with inulin; exceptions were reported in the categories of marine eutrophication and land use, where the bio-based inulin contributed to the majority of the composite impacts. The use of bio-based PBAT implied a reduction in the carbon footprint and fossil resource use of the composite, paired with an increase in marine eutrophication and land use categories highlighting the necessity to consider environmental trade-offs in the evaluation of bio-based alternatives.

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OR08

Development and characterization of lignin-based hydrogels for efficient adsorption and removal of emerging pollutants from aqueous environment

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Water pollution remains one of the most pressing environmental issues of our time. Porous materials are widely investigated for wastewater treatment due to their high specific surface areas that promote effective interactions with target contaminants. However, many such materials are derived from fossil resources and suffer from drawbacks including high cost, non-degradability, and the risk of secondary pollution. Lignin-based porous materials represent a sustainable alternative. Lignin is the second most abundant natural polymer after cellulose and is composed of cross-linked aromatic units—coniferyl, sinapyl, and p-coumaryl alcohols—providing a heterogeneous structure [1]. In this work, acrylamide (AAm) and acryloxyethyltrimethylammonium chloride (DAC) were grafted onto lignosulfonate (LS) in water using potassium persulfate (KPS) and tetramethylethylenediamine (TEMED) as thermal initiator and catalyst at 40 °C, respectively [2]. The resulting cationic hydrogel (LS_pAAm_DAC) was characterized by FTIR to confirm its chemical structure, while SEM, rheology, and TGA analyses were performed to evaluate its morphological, mechanical, and thermal properties. Swelling studies revealed a water uptake of over 1200% after a few hours of immersion. The hydrogel was tested for the adsorption of diclofenac sodium (DCF-Na), an emerging pollutant, through batch and continuous-flow experiments. Batch tests showed high adsorption capacity for an initial DCF-Na concentration of 125 mg/L. Kinetic data followed a pseudo-second-order model, indicating chemisorption via electrostatic interactions. Adsorption isotherms were well described by Langmuir and Sips models, suggesting monolayer coverage and near-homogeneous surface behaviour. Notably, this is the first report of diclofenac removal using a lignin-based hydrogel in a packed-bed column, achieving a maximum capacity of ~50 mg/g. The column data were successfully modelled using Thomas, Yoon–Nelson, and Clark equations.

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OR09

Thermochemical valorization of Chaetomorpha linum from Orbetello lagoon

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Coastal water eutrophication has caused an increase in the biomass of opportunistic macroalgae over the last few decades [1]. The Orbetello lagoon, a brackish closed system in central Italy, has been going through environmental degradation, with climate warming as a major aggravating factor, and hence the gigantic Chaetomorpha linum (C. linum) proliferation dominating over the native species. These abnormally fast-growing seaweeds take in carbon, nutrients, and heavy metals very efficiently, but their accumulation and decay, which are both occurring without control, are sources of organic matter, O_2 depletion, and dystrophic crises [1]. Being low in lignin and high in lipids, C. linum is a resource that is promising for hydrothermal treatment (HT), a process that aims at nutrient recovery and eutrophication alleviation. HT is a thermochemical process that converts wet biomasses into hydrochar, bio-oil, and an aqueous phase (AP) ithout any energy-intensive pre-drying [2].

The reactions take place close to water's critical point ($T_C = 374$ °C, $P_C = 22$ MPa), where it is non-polar [2]. The purpose of this research is to maximize C. linum HT and to determine the nature of the hydrochar and bio-oil as possible sources of fuels or chemicals of higher value. The recover of the energetic and nutritional value from AP is also a source of inspiration.

Figure 1: Thermochemical valorization of *Chaetomorpha linum* from Orbetello lagoon.

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OR10

A New Anilato – based Series of 3D MOFs for Environmental Quality

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Capturing CO_2 from the atmosphere represents a key challenge, since CO_2 has been recognized as the primary anthropogenic greenhouse contributor to the increase of earth's average temperature. Their high porosity, tunable pore size and large surface area make Metal-Organic Frameworks (MOFs) promising candidates to uptake and separate CO_2 from gaseous mixtures. In 2021, some of us synthesized, *via* hydrothermal approach, a new microporous MOF, formulated as $[Co(trz_2An)]n{\cdot}2.5H_2O$ (**CAMOF-1**) [1], by combining 3, 6-*N*-ditriazolyl-2,5-dihydroxy-1,4-benzoquinone as organic linker, with Co^{II} metal node in a 1:1 stoichiometric ratio. This MOF showed a favourable balance of high selectivity, high adsorption capacity and high regenerability, thus being a promising candidate for CO_2 gas separation processes; its framework is capable to sieve larger molecules, such as methane or nitrogen, to reach very high CO_2 selectivity values in different conditions of temperature and concentration. We report herein the synthesis, crystal structure and performance studies of three new microporous MOFs obtained by combining trz_2An with Cu^{II}, Zn^{II} and Fe^{II} metal nodes, formulated as $[Cu(trz_2An)]{\cdot}nH_2O$ **(CAMOF-2),** $Zn(Trz_2An){\cdot}3H_2O$ **(CAMOF-3)** and $Fe(Trz_2An){\cdot}$ $3H_2O$ **(CAMOF-4). CAMOF-2-4,** show a 3D robust structure, with a pore size of 3.46 Å for **CAMOF-2** and 3,89 Å for **CAMOF-3,4,** consistent with the kinetic radius of CO_2 [2] and absorption capacity of 2 molecules of CO_2 / unit formula confirmed by pore analysis data.

Static and Dynamic Adsorption Measurements revealed *i*) remarkable carbon dioxide uptake, *ii)* high selectivity in CO_2:N_2 gas mixtures, *iii)* easy regeneration in mild conditions.

Furthermore, *i)* preliminary CO_2 electroreduction studies showed a good capability of **CAMOF-2** to convert carbon dioxide into ethylene and *ii)* adsorption test removal, performed on **CAMOF-3** and **CAMOF-4,** revealed a good performance to remove Cd^{II}, well known as highly toxic heavy metal ion, at different pH range and concentrations. In conclusion, trz_2An is a strategic organic linker, which combined with different transition metal ions, gave rise to a novel thermal stable, robust, microporous 3D MOFs family employing for environmental quality.

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OR11

Porcine plasma protein-based superabsorbent materials: the influence of salts on the absorption properties

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In recent years, high-porosity materials, such as polyurethane foams, have attracted attention for applications in hygiene, biomedical, agriculture, and food packaging [1,2]. In an effort to replace non-biodegradable plastics with eco-friendly alternatives, this study developed porous composite materials based on porcine plasma proteins (PPP) obtained as by-product of the meat industry. The bioplastics were prepared by blending PPP with glycerol (50 %) and processed by injection moulding at two mould temperatures (60 and 120°C). The effect of three different salts (ammonium bicarbonate, sodium bicarbonate, and sodium carbonate) on absorption properties was evaluated. Chemical-physical, mechanical, and rheological characterizations, along with liquid absorption tests, were carried out. The bioplastic moulded at 60°C with sodium carbonate showed the highest water uptake (3000 ± 200% at 24 h, **Figure 1**), reaching values comparable to a commercial feminine hygiene foam. SEM analysis revealed a complex, interconnected porous structure similar to commercial polyurethane foams. These findings highlight the potential of PPP-based bioplastics as sustainable, high-performance alternatives for industrial applications.

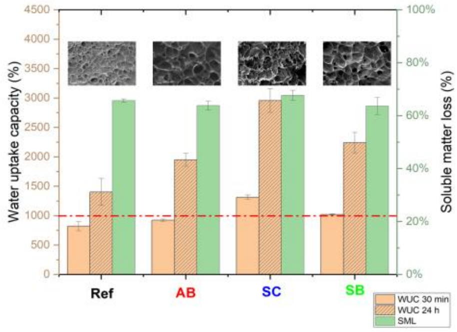

Figure 1: Water uptake (WUC) at 30 min and 24 h, and soluble matter loss (SML) for blends injected at 60 °C without salt (Ref), with ammonium bicarbonate (AB), sodium carbonate (SC), and sodium bicarbonate (SB)

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OR12

Design and synthesis of vanadyl-based molecular qubits using macrocyclic ester ligands

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Qubits are the fundamental units of information in quantum computers. Their optical control and readout are of outstanding importance in the emerging field of quantum technology. This project aims to develop molecular qubits based on half-integer spin metal complexes. Starting from the proper α-substituted malonyl dichloride, a series of macrocyclic ester ligands has been synthesized, purified and characterized by X-ray diffraction. To prepare spin-coherent vanadyl complexes [1] that could act as qubits, complexation experiments with vanadyl nitrate under optimized conditions has been carried out. The evidence for complex formation has been obtained by MALDI experiments. The next step involves the functionalization of the macrocyclic ligand with functional groups suitable for its covalent linkage to fullerene via an azide-alkyne cycloaddition. [2] Fullerene serves as an electron acceptor, a property already exploited in previous studies. [3] This strategy could lead to the development of a molecular antenna which, by photoexcitation and subsequent electron transfer, should provide an unambiguous signal upon detection.

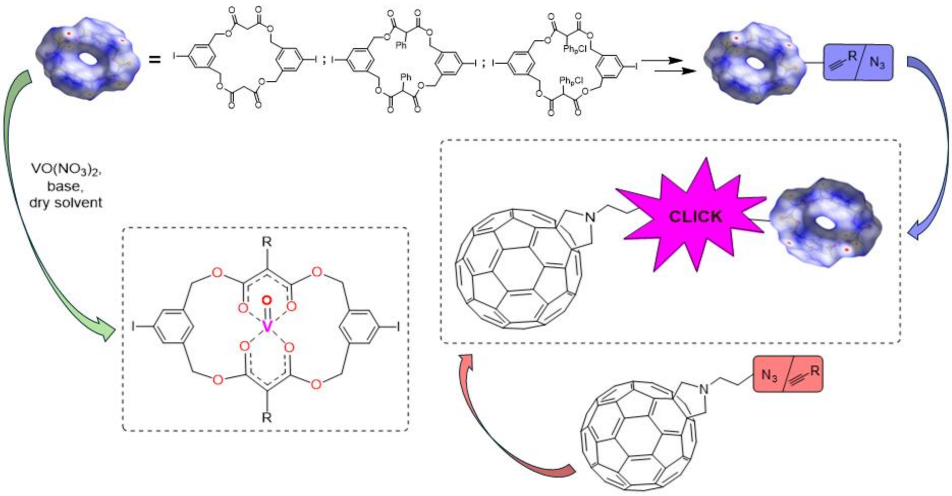

Figure 1: left: complex of vanadyl with macrocycle ligands;
right: click reaction between macrocycle ligands and functionalized fullerene

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OR13

Influence of substituent nature and substitution pattern on spectroscopic properties of a series of new chromogenic and fluorogenic Zn(salmal) complexes

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Zn(salen-type) complexes represent a versatile class of molecular materials, since their spectroscopic properties can be modulated by both the nature of the diimino bridge and the substituents on the salicylidene rings. Among these, Zn(II) complexes derived from 2,3-diaminomaleonitrile — Zn(salmal) — exhibit the most favorable spectroscopic characteristics. Several studies have shown that the fluorescence properties of these complexes depend on both the nature and position of the substituents [1]. However, so far they have been limited to a narrow range of substituent types. Here, we present a systematic study aimed at correlating spectroscopic variations with the electronic nature and positional effects of substituents in a series of chromogenic and fluorogenic Zn(salen-type) complexes, bearing electron-donating and electron-withdrawing groups (NEt_2, OMe, OH, Me, I, Br, Cl, F, NO_2) at the 4- and 5-positions of the salicylidene rings. The electronic effects of these substituents were evaluated by correlating Hammett substituent constants [2] (σ_{para} and σ_{meta}) with experimental data including ^1H NMR chemical shifts, UV–vis absorption maxima, and fluorescence quantum yields, (Φ) [3]. Electron-withdrawing substituents ($\sigma > 0$) induce downfield ^1H NMR shifts and hypsochromic λ_{max} shifts, while electron-donating groups ($\sigma < 0$) lead to upfield ^1H NMR shifts and bathochromic λ_{max} shifts. Notably, 4-substituted Zn(salmal) complexes display a wide range of fluorescence quantum yields (Φ) (from 0.006 for $-NO_2$ to 0.39 for $-NEt_2$), whereas 5-substituted analogues remain weakly emissive ($\Phi < 0.01$) (Figure 1), with the exception of the 5-NO_2 derivative, whose relatively higher Φ suggests additional resonance contributions. Overall, this study provides a reliable quantitative framework to rationalize and predict the electronic effects of substituents in Zn(salen-type) molecular materials, offering a valuable tool for the rational design of molecular materials with tunable photophysical properties

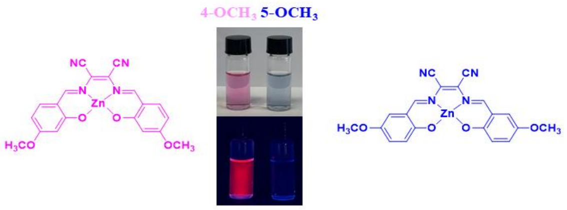

Figure 1: Molecular structures of Zn(salmal)-4OCH_3 (left, magenta) and Zn(salmal)-5OCH_3 (right, blue) and photographs of their relative THF solution 10 μM under natural (top) and 365 nm light (down).

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[3] E. Bobko et al., *J. Org. Chem.* 48, (1983), 1368-1369.

OR14

Detection of mechanical damage in plastics via diarylacetonitrile probes

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The mechanical performance of polymers is crucial across diverse applications, from aerospace to wearable electronics. To better monitor their behavior under stress, optical methods—especially mechanochromic polymers that change color or fluorescence upon deformation—have gained attention for real-time sensing and failure prediction [1]. These materials typically incorporate mechanophores, molecular units that respond to mechanical force via bond cleavage, generating reactive macroradicals [2]. These radicals can trigger further reactions like cross-linking or degradation, impacting material performance. Understanding and tracking radical formation is key to improving the durability and reliability of polymer systems.

In this study, a diarylacetonitrile (DAAN) derivative bearing methoxy substituents in the para position of the aromatic rings was synthesized and investigated as a fluorescent molecular probe for detecting mechanoradicals in commodity plastics such as polyethylene (PE), polypropylene (PP) and Polyvinyl Acetate (PVAc) (Figure 1). DAAN derivatives selectively react with the highly reactive radicals produced during mechanical chain scission, forming relatively stable DAAN-based radical species that exhibit fluorescence under UV light [3]. This property enables the optical detection and spatial mapping of radical formation within stressed polymer matrices, offering a promising strategy for real-time monitoring of mechanical damage at the molecular level.

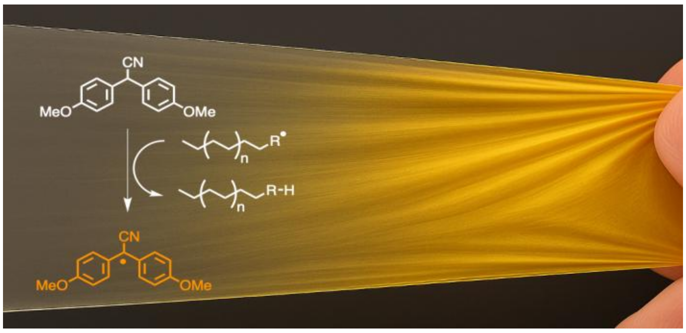

Figure 1: Working mechanism of the mechanochromic polymers.

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OR15

Photon avalanche in metal-organic frameworks: converting infrared light into visible emission and motion

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Upconversion converts two or more low-energy photons into a single photon of higher energy. Among the upconversion mechanisms, photon avalanche (PA) is the most nonlinear one, producing an intense burst of emission once the laser excitation power exceeds a critical threshold. PA has been observed only in lanthanide-doped inorganic matrices where the emission arises from electron accumulation in the 4f levels of lanthanide ions. Applications are in deep-tissue imaging [1]. Here, we generate a broadband PA in lanthanide-trimesate metal-organic frameworks (MOFs) [2]. The PA mechanism is new: PA occurs within the organic molecules. The IR photons are first absorbed and upconverted by a pair of lanthanide ions; then the electrons are funneled into electronically coupled triplet states of the ligand where they accumulate and subsequently are re-emitted (Fig. 1a). The nonlinearity factor is comparable to that of state-of-the-art inorganic PA matrices. Importantly, by selecting different metal ions, the alignment between lanthanide levels and the ligand triplet can be tuned, thus adjusting PA properties. Moreover, the excitation laser pulse features seem to govern the population of diverse vibrational levels of the ligand triplet. Remarkably, preliminary results also showed that IR irradiation triggers a phase change accompanied by microscopic MOF contraction (Fig. 1b), likely due to non-radiative pathways. To our knowledge, this is the first example of IR triggered dynamic crystal. These results broaden PA material design and highlight MOFs as platforms for converting IR light into concurrent controlled motion and intense visible emission.

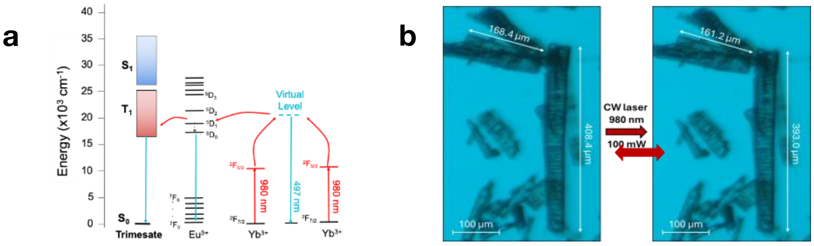

Figure 1: **a** Scheme of the PA mechanism, **b** Optical microscopy images of the crystal before and after IR laser excitation.

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OR16

DNA condensates containing *client* silica nanoparticles (SiNPs) for theranostic applications

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Biomolecular condensates –dynamic, biomolecule-enriched droplets which arise owing to Liquid-Liquid Phase Separation (LLPS) – have been recently described to be implicated in many key vital processes within cells [1]. Although intracellular LLPS is extremely complex, the use of nucleic acids' high programmability, governed by Watson–Crick–Franklin base-pairing, offers a straightforward mechanism to form predictable artificial condensates [1]. Specifically, DNA nanotechnology provides a powerful platform for the engineering of condensates with tuneable structures and functions by capitalizing on the vast toolbox available to the field. Consequently, recent studies have demonstrated the formation of DNA condensates capable of selective-partitioning target molecules of interest, spatiotemporally controlled biochemical reactions and stimuli-responsive phase-separation and partitioning behaviours [2,3].

Herein, we report on the partitioning of mesoporous silica nanoparticles (SiNPs) into DNA-based condensates. Our strategy leverages DNA nanostars as programmable building blocks for condensate formation, which are rationally designed to include an anchoring single-stranded DNA (ssDNA) overhang for the recruitment and local concentration of SiNPs functionalized with complementary DNA sequences. To explore the parameters governing nanoparticle partitioning, we constructed a toolbox of SiNPs varying in size (from 90 to 700 nm) and surface chemistry (DBCO-modified and carboxylated), allowing us to investigate the combined effects of particle size, surface properties, and sequence-specific hybridization on partitioning behaviour within the condensate. Our findings indicate that there is no strict size threshold limiting SiNP partitioning into DNA condensates and provide insights into how biomolecular condensates mediate selective client loading and molecular interactions. Future work will involve using these hybrid DNA-SiNPs condensates decorated with responsive aptamer moieties for cellular targeting and smart release capabilities, where SiNPs may be used to load therapeutic drugs and DNA condensates will act as biocompatible molecular shells which can be designed to be stimuli responsive.

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OR17

Nanostructured luminescent biomaterials from organic dyes and diatom frustules

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Diatoms, a highly diverse class of photosynthetic unicellular microalgae, are among the most promising living organisms for generating nanostructured components. Their mesoporous silica shells (frustules) offer a unique combination of high surface area, mechanical strength and distinctive optical features, making them ideal candidates for a wide range of advanced applications [1]. The outstanding potential of biosilica in nanotechnology is due to its porosity and the presence of surface hydroxyl groups, which provide reactive sites for targeted chemical functionalization. In particular, our study highlights several strategies, including physisorption, covalent bonding and polymer incorporation, for functionalization of diatom frustules with photoactive organic molecules [2]. The interaction between the transparent silica matrix and the photoluminescent properties of the incorporated molecules enables the development of new bioderived hybrid materials. These engineered structures open up exciting opportunities in biomedicine, optics and photonics [3].

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OR18

Supramolecular Gels from Lipoamino Acids: study and applications

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Supramolecular gels are a class of materials in which gelators self-assemble in fibrillar networks, due to non-covalent interactions, after the addition of a trigger (pH, solvent, ultrasounds, temperature). Among many low molecular weight gelators, lipoamino acids have shown interesting gelling properties.

Their structure is characterized by an aminoacidic residue and a long aliphatic side chain. Depending on the aminoacidic residue it is possible to exploit different interactions (electrostatic, hydrophobic, π-stacking, hydrogen bonding), and the aliphatic chains of the fatty acid may contribute through Van der Waals interactions.

This research project evaluates a new acidic trigger, Acetyl Valine [1], on previously studied lipoamino acids gelators: Pal-L-Phe-OH [2] and Lau-L-dopa$(Bn)_2$-OH [3]. Ac-Val was added to gelator solutions in volume, causing an instantaneous pH modification. It was proved that Ac-Val, compared to GdL (solid) and commercial lactic acid solution, offer many advantages: it is fully water-soluble, overcoming dissolution problems; enables the preparation of a stock solution at a specific pH value. Stock solutions are less accurate for lactic acid because the commercial solutions lack a defined concentration. Gels have been characterized with rheometer, SEM, X-ray powder diffraction and ATR-IR, showing that Ac-Val forms homogeneous and reproducible hydrogels. The tunability of the pH allows the preparation of hydrogel from 4.0 to 6.5, making them suitable both for cosmetic and biomedical (drug delivery) applications.

In the cosmetic field lipoamino acids gelators can be used as rheological modifiers in emulsions, instead of synthetic acrylate, being able to form supramolecular structures in oil and water phases, modifying the viscosity of the emulsion and leading to the formation of more biodegradable and sustainable products.

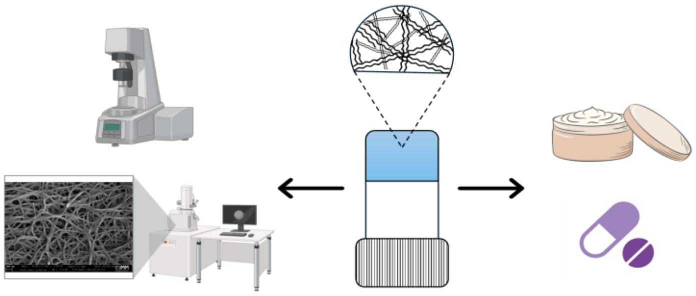

Figure 1: Characterization and applications of supramolecular hydrogels.

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OR19

Direct Ink Writing of Methyl Methacrylate and Styrene via Tailored High Internal Phase Emulsions

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We present a new strategy to 3D print organic monomers such as methyl methacrylate (MMA) and styrene via Direct Ink Writing (DIW). Unlike Fused Deposition Modeling (FDM), where thermoplastic polymers are extruded in the molten state, DIW allows materials to be deposited and subsequently polymerized, enabling the processing of thermosetting systems. However, common organic monomers such as MMA and styrene are generally unsuitable for DIW due to their Newtonian rheological behavior and limited reactivity under UV-induced radical polymerization.

To overcome these limitations, we formulated two High Internal Phase Emulsions (HIPEs) of the oil-in-water type: one with an organic phase based on methacrylic monomers and a crosslinker, and another with styrene and divinylbenzene. A thermal radical initiator was incorporated into both organic phases. In the aqueous phase, chitosan methacrylate and a photo radical initiator were included, enabling rapid immobilization of the structure immediately upon UV exposure during printing. Subsequent curing of the organic phase was carried out in an oven.

Prior to printing, rheological analyses confirmed the printability of the emulsions, which were also morphologically investigated using confocal microscopy. Printing tests were performed to correlate print quality with printing speed and extrusion pressure. Mechanical tests were conducted on the printed structures and compared with both bulk-polymerized emulsions and bulk-polymerized neat organic phases. Finally, several demonstrative objects were fabricated, showcasing the good printing fidelity of the emulsions.

These systems are promising not only because they enable the use of various organic monomers, but also because they can form stable foams. This makes them particularly attractive for the 3D printing of materials with tailored porosity gradients.

OR20

Exploring the role of amino-functionalised nanocellulose materials as organocatalysts and metal-coordinating scaffolds

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In recent years, both industry and academia have strongly pursued the concept of green and sustainable chemistry, especially in the field of catalysis. However, a current issue is the use of amine-containing organocatalysts, that are mostly employed in the homogeneous phase, with difficult separation steps and a high amount of waste. State-of-art heterogeneous catalysts are currently designed for an environmentally friendly purposes, aiming at easier recovery, biodegradability and recyclability of all the materials involved [1]. One great option for supporting active molecules are biopolymers, because of the flexibility they offer in terms of structure [2]. Particularly, cellulose and its nanosized derivatives have already been investigated as scaffolds for nanoparticles (NPs), that nowadays are a widespread method to perform crucial metal-catalysed reactions in chemical engineering [3]. NPs offer several advantages, such as high surface area and ease of access for reagents, but they also suffer from slower reactivity with respect to their homogeneous counterparts.

To overcome these issues, in this work we first extracted cellulose nanofibers (CNFs) with chemical and mechanical methods, and we functionalised them with amino groups, thus developing an engineered nanocellulose material with dual ability: by itself, for amino-catalysed reactions, and as a coordinating agent for metal ions. In this way, we were able to turn an inert polymeric scaffold into an active participant in several reactions. Finally, we tested the reactivity of our homogeneous-inspired heterogeneous catalysts obtaining excellent yields for both organocatalysis and metal-driven reactions, highlighting the potential of a new perspective on nanocellulose-based catalysts.

Figure 1: Graphical abstract

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OR21

Lanthanide-based porphyrazine derivatives: chemico-physical properties and potential applications in biomedicine

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In our previous extensive studies the synthesis, chemico-physical properties and photoactivity as anticancer drugs in photodynamic therapy (PDT) [1] were reported of mononuclear octa(2-pyridyl)tetrapyrazinoporphyrazines complexes, having centrally coordinated trivalent diamagnetic metals, formulated as $[Py_8TPyzPzMX]\cdot xH_2O$ where $Py_8TPyzPz$ = tetrakis-2,3-[5,6-di(2-pyridyl)pyrazino]porphyrazine and MX = $Al^{III}Cl/OH$, $Ga^{III}Cl/OH$, $In^{III}OAc$ (Cl = chloride anion; OH = hydroxide anion; OAc = acetate anion) (Figure 1A). For the obtained compounds the photosensitizer activity for the generation of singlet oxygen, $^1O_2$, the main cytotoxic agent in PDT, was explored in DMF and DMF/HCl solutions. These species have high quantum yield values (Φ_Δ = 0.5-0.7) which are higher than those obtained for the series $[Py_8TPyzPzM]$ (M = Zn^{II}, $Mg^{II}(H_2O)$, Pd^{II}, Pt^{II}) [2].

In a recent extension of our work on TPyzPzs it was thought interesting to undertake additional studies on new porphyrazine metal derivatives with trivalent metals of lanthanide series, with the aim of examining their potential applications in biomedical field [3]. New mononuclear tetrapyrazinoporphyrazine complexes having centrally coordinated Nd^{III}, Yb^{III} and Lu^{III}, formulated as $[Py_8TPyzPzM(OAc)]\cdot xH_2O$ (M = Nd^{III}, Yb^{III}, Lu^{III}) (Figure 1B), have been synthesized and characterized, exploring in particular their magnetic behavior which depends on several factors such as the nature of the metal ion. For all three complexes the photosensitizing activity for the generation of singlet oxygen was explored in DMF and in DMF/HCl. The high Φ_Δ value obtained for the Lu^{III} macrocycle in DMF/HCl solution (0.86) is considerably higher than those observed for numerous porphyrazines. This result qualifies the Lu^{III} complex as an excellent photosensitizer for the generation of $^1O_2$, with the perspective of being used as a potential anticancer agent in PDT.

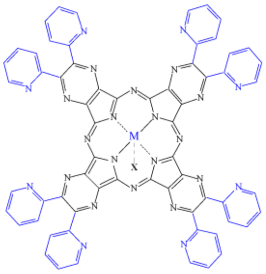

Figure 1A

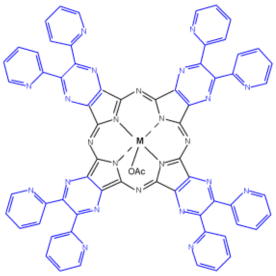

Figure 1B

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OR22

Aldehydes as CO releasing molecules: in-situ and ex-situ Giese reactions and Palladium catalyzed aminocarbonylations

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Carbon monoxide (CO) represents a fundamental C1 synthon, widely utilized in several carbonylation reactions. Its hazardous nature, however, has made necessary the development of proper strategies for its safe manipulation, e.g. the use of stable CO precursors, known as CORMs (CO-releasing molecules) [1,2].

These surrogates allow for a smooth, controlled release of CO – whether through thermal or photochemical activation – within the reaction mixture. The decarbonylative process, however, generates various undesired byproducts (deriving from the residual fragments of the CORMs), resulting in a poor atom economy.

In our work, we addressed this drawback by adopting a two-chambers reactor (**Figure 1a**). In Chamber A, the CORM, i.e. a proper aldehyde, is activated, upon light irradiation at 390 nm, by a decatungstate (TBADT)-photocatalyzed hydrogen atom transfer, to the corresponding acyl radical, which spontaneously decarbonylate, releasing an alkyl radical. The latter undergoes a Giese reaction, via conjugate addition onto a Michael acceptor, while the photogenerated carbon monoxide, once reached Chamber B, is exploited in the Palladium photocatalyzed aminocarbonylation of an aryl iodide triggered by the same wavelength (390 nm) [3].

Both types of reactions showed a remarkable efficiency, allowing to obtain several Giese adducts and benzamides in good yields, and assuring a full incorporation of the CORM structure in the final products.

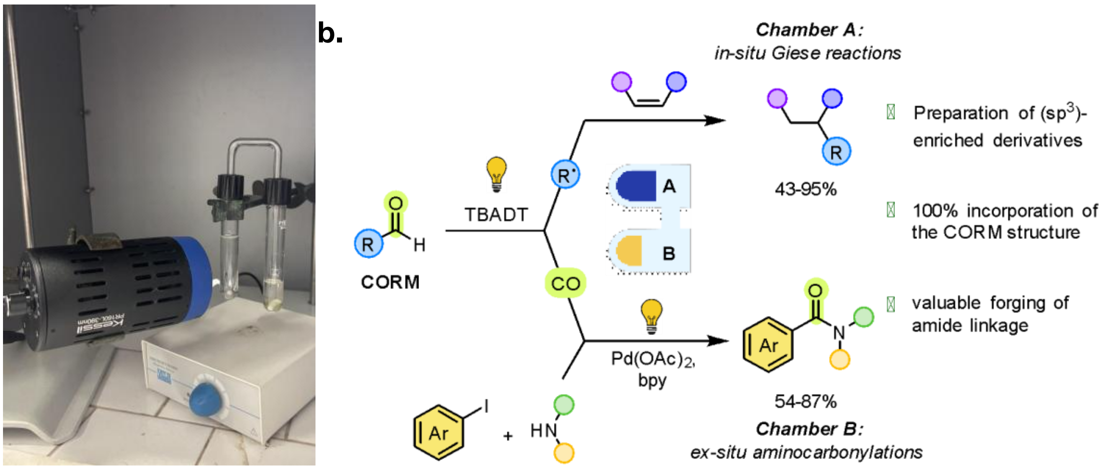

Figure 1: **a.** Two chambers setup employed for the reaction (Chamber A on the left, Chamber B on the right) **b.** Aldehydes as CORMs

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OR23

Halide-Rich $Cs_3Bi_2Br_9$ Nanocrystals as Efficient Photocatalysts for Visible-Light-Driven Benzyl Alcohol Oxidation

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The design of sustainable photocatalysts for selective alcohol oxidation remains a major challenge in green chemistry [1]. Here, we introduce a ligand-assisted reprecipitation (LARP) strategy that affords halide-rich $Cs_3Bi_2Br_9$ nanocrystals with unprecedented control over size, morphology, and surface composition. Excess halide suppresses particle growth during synthesis, and its removal in subsequent washing steps exposes catalytically active bismuth sites [2]. Under visible-light irradiation in air, these nanocrystals deliver a record benzaldehyde formation rate of 14500 μmol g^{-1} h^{-1}, nearly one order of magnitude higher than bulk $Cs_3Bi_2Br_9$. Beyond benchmark activity, the catalyst demonstrates broad versatility across different benzylic and secondary alcohols, highlighting its potential for general oxidative transformations. Mechanistic studies and theoretical calculations reveal that surface halide stoichiometry governs the balance between superoxide-driven oxidation and competing pathways. This work establishes a scalable and lead-free platform for engineering high-performance perovskite-inspired photocatalysts for sustainable organic synthesis.

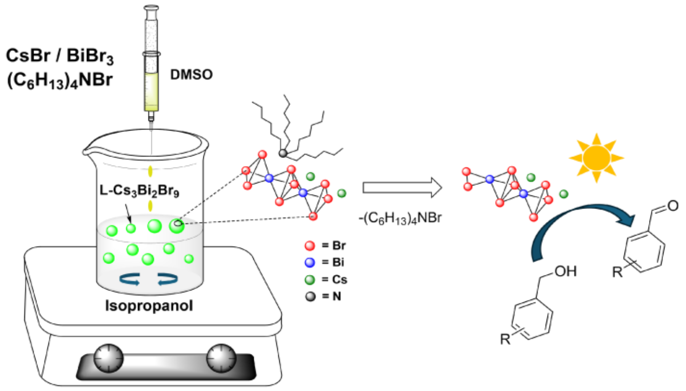

Figure 1: Surface-tuned $Cs_3Bi_2Br_9$ (LARP) catalyses benzyl alcohols oxidation.

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OR24

Role of Cyclic Carbonates in Enhancing UV-Cured PEO–PEC Electrolytes for Room Temperature Lithium Metal Batteries

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Solid-state lithium-metal batteries (SSLMBs) hold promise for next-generation energy storage by combining high energy density with improved safety using non-flammable, low-volatility electrolytes. However, their widespread adoption is limited by low ionic conductivity, sluggish Li^+ transport, and poor interfacial stability of solid polymer electrolytes (SPEs) at room temperature. Poly(ethylene oxide) (PEO), while effective in coordinating Li^+ ions, suffers from high crystallinity and limited conductivity at ambient conditions. To address these challenges, we designed a solvent-free, UV-cured PEO-poly(ethylene carbonate) (PEC) matrix, leveraging PEO's ion-solvating ability and PEC's amorphous, mechanically robust character [1],[2].

To further enhance conductivity and interfacial performance, cyclic carbonate plasticizers—ethylene carbonate (EC), propylene carbonate (PC), and 1,2-butylene carbonate (BC)—were incorporated into the PEO–PEC network. These additives reduce the glass transition temperature, enhance chain mobility, and improve Li^+ solvation, thereby facilitating uniform ion-conduction pathways. Comprehensive electrochemical, thermal, and mechanical analyses reveal that BC-containing systems, in particular, suppress crystallinity, increase amorphous content, and provide stable compatibility with lithium metal [3]. The optimized SPEs exhibited high oxidative stability and enabled reversible cycling in Li plating/stripping as well as in full-cell configurations (LFP and NMC622) at room temperature. Our findings demonstrate a rational additive-engineering strategy for UV-cured PEO-PEC electrolytes, offering an effective pathway to overcome the conductivity and stability challenges of solid-state systems.

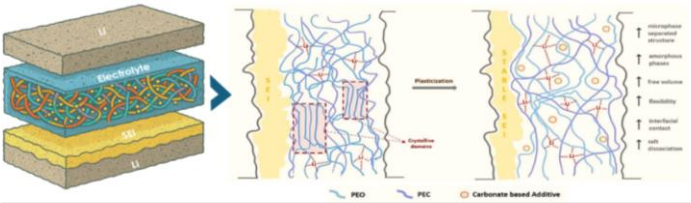

Figure 1: Schematic representation of the effect of plasticizers on SPEs.

Acknowledgements: This study is supported by the MSCA-funded European Union project RIDERS (GA 101120432), in collaboration with Blue Solutions and the Horizon EU project PSIONIC (GA 101069703).

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OR25

Transient changes in conductivity of a water solution by means of an activated carboxylic acid

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Dissipative chemical systems, in which chemical or photophysical stimuli are consumed to maintain a nonequilibrium (and hopefully functional) state, are currently the object of intense investigation. In this context, activated carboxylic acids (ACAs) have been extensively used as chemical stimuli to drive a vast number of different acid-base-responsive dissipative systems [1].

Nowadays, an interesting area of research is represented by the development of ACA-powered systems in which the expressed phenomenon is not, per se, acid-base in nature. We recently showed that ACAs can be used to control non-pH-responsive devices via signal transduction [2].

Here, we investigated the possibility of using nitroacetic acid to control, over time, the electrical conductivity of an aqueous solution. In this case, the addition of the ACA directly affects the conductivity of the solution, removing the need for a signal transductor. The aqueous solution must be initially characterized by a very low ion content, thus a low electrical conductivity. The addition of nitroacetic acid produces an immediate and remarkable increase in conductivity, which persists until the acid is entirely consumed by the system. Varying the experimental conditions in which the measurements are performed allowed us to control the time required for the system to return to the low conductivity state, and to tune the maximum conductivity value reached by the system. We then interfaced this newly designed dissipative system with simple electric circuits, where it behaved as a chemically driven variable resistor.

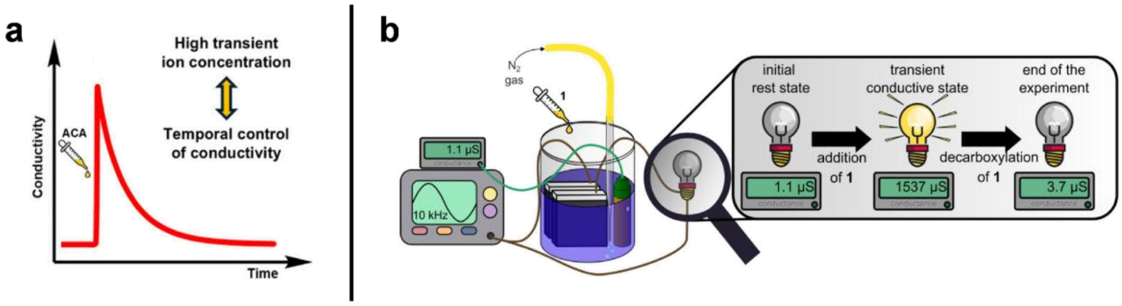

Figure 1: a) Typical conductivity profile of the aqueous solution after the addition of nitroacetic acid. b) Pictorial representation of the circuit involving the system as a variable resistor.

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OR26

Development and validation of an UHPLC-FLD method for the monitoring of BPA and BPF in infant milk

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Bisphenols (BPs) are synthetic compounds widely used in the manufacture of many plastic items, including food packaging, and recognized as endocrine-disrupting chemicals [1]. Their contamination can occur during all the stages of food production chain. Due to the heightened vulnerability of newborns to chemical contaminants, monitoring BP levels in infant foods is a major public health priority. In this study, outlined in Figure 1, an analytical procedure was *in-house* developed and validated according to the Eurachem (2025) guidelines for the quantification of bisphenol A (BPA) and bisphenol F (BPF) in infant milk products. This method consists of a QuEChERS-based extraction and clean-up and an Ultra-High Performance Liquid Chromatography coupled with Fluorescence Detection (UHPLC-FLD) analysis [2]. Fluorescence detection proved to be well-suited for the analysis of BPs due to the high sensitivity of the method (LOQs = 1.56 ppb), which also provided reliable results in terms of trueness (recoveries ranging from 86.78% to 95.00%) and precision as repeatability and intermediate precision ($RSD_r \leq 8.34\%$ and $RSD_R \leq 8.42\%$). For these reasons, the proposed method has proven to be suitable and reliable for routine analysis of BP traces in infant milk formula.

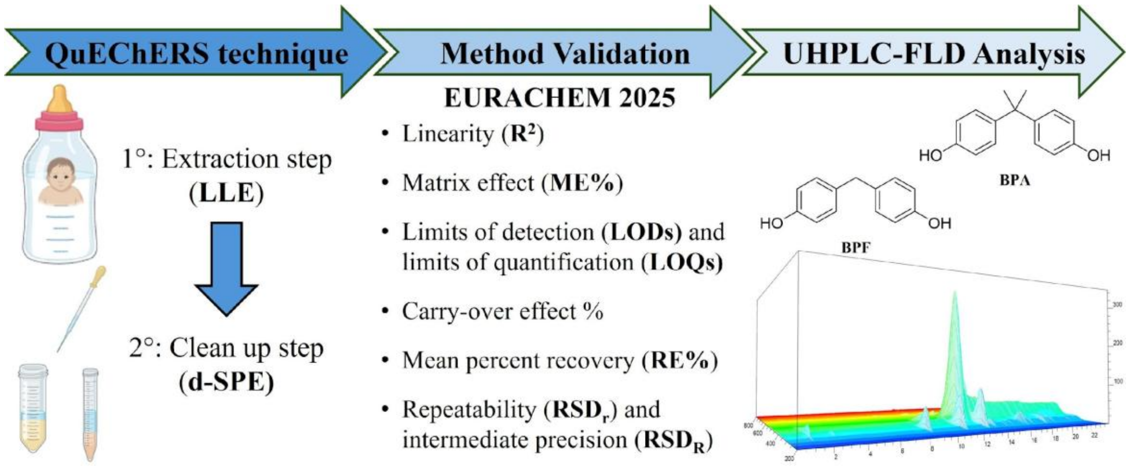

Figure 1: Experimental workflow of this study.

[1] N. Caballero-Casero, L. Lunar, and S. Rubio, *Anal. Chim. Acta.* 908 (2016) 22-53.
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OR27

Tracing the aging of Italian balsamic vinegars through compound-specific isotope analysis

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Stable isotope analysis represents a powerful approach for assessing food authenticity and geographical origin, particularly in products with geographical indications [1]. Among these, Aceto Balsamico Tradizionale di Modena (ABTM, PDO) and Aceto Balsamico di Modena (ABM, PGI) are of great interest due to their high cultural and economic value. Understanding how aging affects the isotopic composition of individual compounds is crucial for distinguishing traditional from non-traditional products and strengthening authenticity verification.

In this work, the aging process of Italian balsamic vinegars was investigated by monitoring $\delta^{18}O$ in water and $\delta^{13}C$ in glucose, fructose, and acetic acid. In addition, bulk parameters such as water content, density, total acidity, refractive index, and sugar concentrations were evaluated to complement isotopic data. The results revealed a progressive increase of $\delta^{18}O$ values of water along the aging process in ABTM cask series, providing a reliable marker for differentiating traditional from non-traditional balsamic vinegars. Conversely, $\delta^{13}C$ values of glucose, fructose, and acetic acid were influenced not only by aging but also by the origin of raw materials and production conditions. These findings demonstrate the potential of compound-specific isotope analysis to trace the aging process of balsamic vinegar and contribute to its authentication, while also highlighting the need for further research to disentangle the multiple factors affecting $\delta^{13}C$ variations.

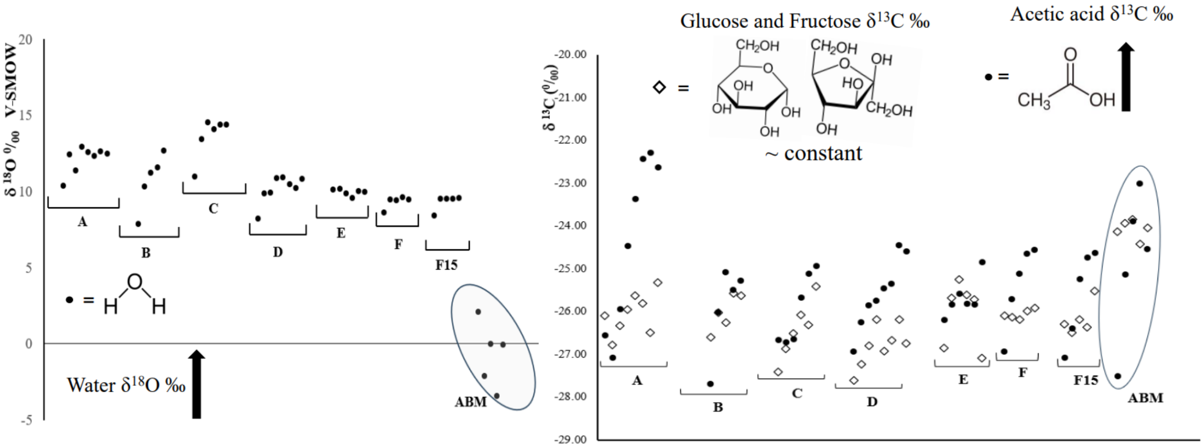

Figure 1: $\delta^{18}O$ values of water during the aging process of ABTM (left); $\delta^{13}C$ values of glucose, fructose, and acetic acid in ABTM (right), both compared with the corresponding isotopic data of ABM.

[1] L. Lancelllotti, V. D’Eusanio, D. Manzini, C. Durante, A. Marchetti, and L. Tassi, *Foods.* Ed. 14 (2025) 9-1492

OR28

Chemometric Analysis of Durum Wheat Using Portable NIR Spectrometers: Effects of Acquisition Mode and Instrumental Variability

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Portable spectroscopic sensors that operate in the Near-Infrared (NIR) spectrum are gaining momentum across both research and practical domains. This growing interest is largely due to their cost-effectiveness, user-friendly interface, and the technological progress that has led to the creation of compact yet high-performance devices. In contrast to traditional benchtop spectrometers, portable instruments enable direct, on-site analysis, which simplifies the workflow and reduces turnaround time. Ongoing innovations in both hardware and software have broadened the range of potential applications for these sensors in several fields [1].

Nonetheless, these instruments come with specific limitations, including a narrower spectral coverage, limited operational versatility, and heightened sensitivity to environmental and procedural conditions. Therefore, they should be recognized not as mere scaled-down laboratory tools, but rather as analytical devices with distinct features and methodological considerations [2].

The present study investigated the NeoSpectra portable NIR scanner, which operates within the 1250–2500 nm range, to evaluate its capability to predict protein and moisture content in a dataset of 103 wheat samples sourced from various Italian regions. Analyses were performed on intact, untreated kernels, under varying operational setups. These included differences in power supply (battery versus charging), frequency of background collection (before every scan versus once per session), measurement strategy (static point-based versus rotary), and number of independent analytical sessions.

To ensure data quality, spectral signals underwent pre-processing aimed at noise reduction and outlier detection. Subsequently, predictive models were constructed using advanced multivariate chemometric techniques [3].

The results clearly indicate that the tested sources of variability significantly impact the predictive accuracy of the models. This highlights the necessity of a well-structured experimental design when building robust and generalizable calibration models. Thanks to their capacity for non-destructive, in-field analysis of unprocessed materials, portable NIR sensors represent a promising solution for rapid quality control in the agri-food industry. When combined with chemometric tools, NIR spectroscopy offers an efficient and reliable pathway for assessing key compositional parameters in agricultural products.

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OR29

Modulation of aroma release in industrial ice cream through hydrocolloid blends

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Flavor perception in frozen desserts is influenced not only by the composition of odor compounds but also by the structural properties of the food matrix, which controls their release during consumption. Stabilizers, widely used to control ice cream texture and stability, can modify ice cream's melted phase (serum) viscosity, ice crystal structure, and melting behavior, thereby affecting odor compound delivery [1,2]. In this study, eleven stabilizer blends, including locust bean, guar, alginate, xanthan, cassia gum, and κ-carrageenan, were evaluated for their effect on the release of different volatile organic compounds (i.e., esters, alcohols, terpenoids, and lactones). The effect was also verified under different storage conditions.

Ice creams were produced in a pilot plant at 100% overrun and stored at -12°C and -20°C for six months. Aroma release was monitored by Proton Transfer Reaction Mass Spectrometry (PTR-MS), during ice cream melting and in model systems.

Blends with higher serum viscosities (≈ 59.644 mPas), such as Alginate (A) and Guar+Alginate+κ-carrageenan(GAK), showed significantly reduced volatile compound loss, the decrease in headspace concentration of odor compounds during melting, compared to the industrial reference ($p < 0.05$). Storage at −12°C resulted in greater aroma losses than at −20°C, highlighting the role of temperature in stability. PCA supported these findings (Figure 1), with alginate-rich systems clustered away from the reference, suggesting that higher viscosity is linked to reduced aroma loss

Overall, both formulation and storage temperature strongly influence aroma stability in ice cream, with matrix structuring playing a key role in aroma retention.

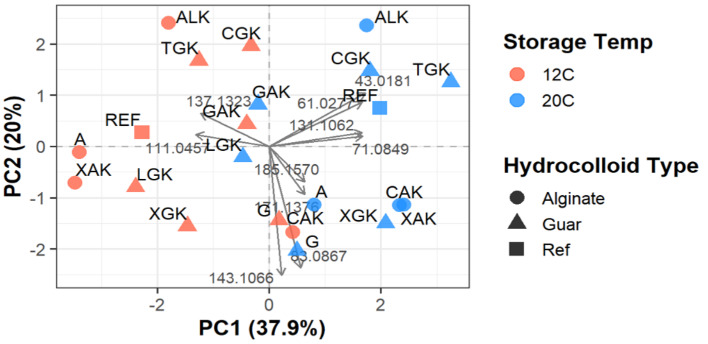

Figure 1: Principal Component Analysis (PC1 = 37.9%, PC2 = 20%) of volatile release profiles in ice cream formulations

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OR30

Development of an integrated analytical system for the analysis of chiral and achiral pesticides in food

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A novel analytical system was developed for the determination of both chiral and achiral pesticide residues in food matrices. The innovative set up integrates two chromatographic techniques: comprehensive two-dimensional enantio-gas chromatography combined with low-pressure GC-MS (eGC×LP-GC-QMS), and low-pressure GC-MS (LP-GC-QMS). A key feature of the system is a switching valve, which increases flexibility, robustness and enables backflushing of the chiral column in the first dimension (max. 230 °C), improving matrix co-extracts removal. The need of perform an enantiomeric separation and monitor the residue pesticides is essential for guarantee the food safety. Furthermore, chiral pesticides can exhibit different activity against parasites, have a different biodegradation or can be toxic to human in one form but not the other. Considering the significant differences between enantiomers, enantiomeric separation is necessary in correctly assessing the potential health risk of eating contaminated food. For this reason, the method was successfully applied to both chiral and achiral pesticide analysis. The first dimension allows enantiomeric separation, while the second - a wide-bore column (5 m × 0.53 mm ID × 0.53 µm) under vacuum - supports high-temperature operation (up to 320 °C), expanding the range of detectable pesticides. The system requires no hardware modifications between applications, making it well-suitable for routine monitoring of pesticide residues in food.

Acknowledgments The authors thank Shimadzu Corporation and Merck Life Science for their support.

OR31

Enriched glucosinolate-extracts from radish microgreens as novel nutraceuticals with antihypertensive potential

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Microgreens are emerging as sustainable biofactories for the standardized production of bioactive compounds with nutraceutical applications. Among these, radish (*Raphanus sativus* L.) microgreens are particularly rich in glucosinolates (GSLs), sulfur-containing secondary metabolites that have gained attention for their ability to act as hydrogen sulfide (H_2S) donors, and as consequence contributing to blood pressure regulation [1,2].

Seven radish cultivars (Red Giant, Saxa, White Tip, Daikon, Red Rubin, China Rose, Tango) were cultivated under controlled hydroponic conditions and harvested after 6, 9, or 12 days. GSLs were extracted, characterized and quantified by HPLC-HESI-MS/MS, while total polyphenols and anthocyanins were determined by spectrophotometric assays. The qualitative polyphenols and anthocyanins profiling was performed by HPLC-HESI-MS/MS. Antioxidant activity was evaluated by DPPH and ABTS methods. Food-grade aqueous extractions were employed to ensure suitability for nutraceutical applications. Their efficiency was assessed through recovery studies, which yielded values close to 100%. The Saxa cultivar, harvested at day 9, exhibited the highest total GSL concentration (101.94 mg of total GSLs/g of dry weight), together with significant antioxidant capacity (DPPH IC_{50}: 1.2 mg/mL; ABTS IC_{50}: 0.67 mg/mL), and relevant contents of phenolics (7.17 ± 0.29 mg Gallic Acid Equivalents/g of dry weight) and anthocyanins (1.71 ± 0.58 mg Cyanidin-3-glucoside Equivalents/g of dry weight).

Moreover, aqueous extracts of 9-day-old Saxa microgreens demonstrated the ability to release H_2S in a concentration-dependent manner (up to 30 mM from 3 mg/mL of aqueous extract) and induced a significant vasorelaxant effect on pre-contracted rat aortic rings (maximum effect at 200 µg/mL, $^{****}p < 0.0001$ vs vehicle).

These findings highlight radish microgreens as a promising source of standardized bioactive compounds, supporting their dual role as antioxidants and natural antihypertensive agents, and reinforcing their value as novel ingredient for nutraceutical formulations.

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OR32

Antagonists and inverse agonists efficacy at A_{2A} adenosine receptors in comparison for the treatment of colorectal cancer

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Decreased efficacy of many agents *in vivo* is often related to alterations in cellular dynamics and poor drug penetration into solid tumors. The compound 9-ethyl-8-(furan-2-yl)-2-(4-methoxyphenethyl)-9H-purine-2,6-diamine (compound **1**), selected from the in-house library for its A_{2A}AR strong affinity and selectivity, was *in vitro* studied in CRC cell lines (Caco-2, HCT116). This compound significantly reduced the viability of tumor cell lines in a concentration-dependent manner.

Caco-2 and HCT116 three-dimensional (3D) spheroids were generated. Since optimized organoid conditions (coefficient of variation 5%, diameter 500 µm) were established as solid tumor models, only spheroids that respect these parameters were selected. Caco-2 and HCT116 spheroids showed approximately two-fold greater resistance to compound **1** than their 2D cultured counterparts (131 and 207 µM versus 72 and 59 µM, respectively), overcoming the well-known five-fold loss of potency of cisplatin in 3D models [2].

Although structurally similar to **ZM241385**, compound **1** is three orders of magnitude less potent as an inverse agonist (4186 ± 1295 nM versus 7.9 ± 0.6 nM), but approximately 30% more potent as an antagonist (131 ± 16 nM versus 187 ± 29 nM). This suggests that antagonism mainly determines antitumor activity, with inverse agonism playing a minor role, contrary to what is observed in Parkinson's disease models [3]. Differences in receptor modulation may influence the cell death pathway: inverse agonists induce necrosis through complete suppression of basal cAMP, while antagonists selectively disrupt adenosine signaling with potentially fewer off-target effects. The results of the FITC-Annexin V/PI assay support this hypothesis, showing that apoptotic cell death is more dominant following treatment with compound **1** compared to **ZM241385** and this difference is even more pronounced in 3D models compared to 2D cell monolayers.

Overall, our data establishes A_{2A}AR as a promising target in CRC and highlights the potent apoptotic activity of compound **1** as an A_{2A}AR antagonist, in contrast to the more pro-necrotic effect of **ZM241385** observed in colorectal spheroid tumor models. These findings make A_{2A}AR antagonism a promising approach for the treatment of solid colorectal tumors.

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OR33

Nanoparticle-mediated delivery of novel MbtI Inhibitors as an anti-virulence strategy against *Mycobacterium tuberculosis*

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Tuberculosis (TB) is the leading cause of death from a single infectious agent and remains a major global health challenge. According to the World Health Organization (WHO), approximately 10 million new cases and 1.4 million deaths are reported annually. In addition, the emergence and spread of multi-drug-resistant strains of *Mycobacterium tuberculosis* (*Mtb*) highlight the urgent need for new therapeutic strategies [1]. In our efforts to address this global threat, we have focused on anti-virulence agents as an innovative therapeutic approach. Within this context, targeting iron acquisition is particularly attractive, as iron is an essential cofactor for the establishment and persistence of mycobacterial infection. Our group performed a classical medicinal chemistry approach to develop inhibitors of MbtI, the first enzyme in the mycobacterial siderophore biosynthetic pathway, which is essential for iron uptake. Our efforts led to the identification of 5-(3-cyano-5-isobutoxyphenyl)furan-2-carboxylic acid (compound **1**) as a potent enzymatic inhibitor of MbtI. Considering the challenges of TB treatment, we investigated the use of nanoparticles to improve drug delivery, aiming for safer and more effective formulations. We encapsulated the ethyl and propyl ester derivatives of compound **1** (**1a** and **1b**) into PMPC-PDPA polymersomes (POs) able to selectively target the macrophages. The resulting POs were fully characterized, and MTT assays confirmed the absence of cytotoxicity for both the free compounds and the encapsulated formulations. Furthermore, we demonstrated that the prodrugs **1a** and **1b** can be efficiently converted into the active acid form by hydrolase enzymes. Finally, fluorescence-based activity assays on murine alveolar-like macrophages infected with *Mtb* showed that drug-loaded POs effectively reduce *Mtb* virulence, with the strongest effect observed one day post-treatment [2].

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OR34

Refactored M13 phage bioconjugates: a novel platform for precision cancer therapy

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Modern anticancer treatments are focused on maximizing therapeutic efficacy while minimizing systemic toxicity. Targeted therapies, particularly Antibody-Drug Conjugates (ADCs), have demonstrated the ability to selectively deliver chemotherapeutic agents to malignant cells, thereby improving clinical outcomes and patient quality of life [1]. However, ADCs remain limited by the reduction of biorecognition ability toward the biological target and limited physiological stability upon drug conjugation, restricting their overall therapeutic index.

Refactored bacteriophages are a innovative biotechnological platform designed for targeted delivery of therapeutic agents. Using an orthogonal strategy, bacteriophages can be genetically engineered to display diverse targeting moieties (e.g., nanobodies) on their capsid minor proteins, while allowing chemical conjugation of a high payload of anticancer molecules on their capsid major coat protein [2].

In this work, we engineered M13 phages, via Phage Display, to target epidermal growth factor receptors — a class of receptors frequently overexpressed in various solid tumors. The engineered phages were further purified and bioconjugated with a high payload of cytotoxic agents using both cleavable and non-cleavable linkers. This approach yielded a drug-to-phage ratio two orders of magnitude greater than conventional ADC platforms, potentially enabling superior intracellular drug release and enhanced antitumor efficacy.

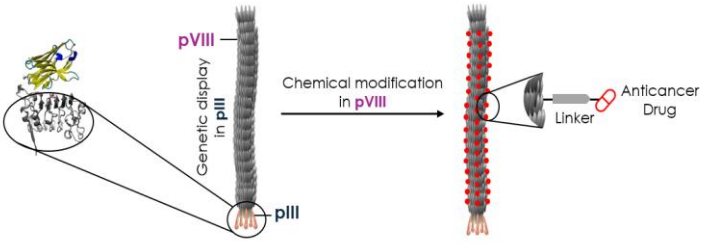

Figure 1: Schematic representation of the project.

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OR35

Development of gold nanoparticles functionalized with peptides to target peri-synaptic integrin receptors αVβ3

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Several treatment-resistant brain disorders, such as stroke and epilepsy are characterized by dysfunctional or damaged synaptic connectivity. It has been proposed that applying a mechanical stimulus to peri-synaptic mechanoreceptors such as the αVβ3 integrin receptor may be an innovative approach to restore physiological synaptic connectivity. To test this hypothesis, we aim at developing nanoparticles that target selectively αVβ3 integrins in the context of in vitro neuronal cultures. In this contribution, we present our strategy to prepare spherical gold nanoparticles (AuNPs) of approx.. 40 nm diameter functionalized with an αVβ3 selective ligand based on the known peptide sequence RGD included into a cyclic pseudopeptide [1]. We also developed AuNPs displaying an analogous ligand with the sequence RAD as negative controls. Additionally, all our AuNPs carry the far-red fluorophore SiR allowing fluorescence microscopy investigations. We will show that the developed AuNPs indeed target the αVβ3 integrins and discuss their effect on cultured neurons. Finally, we will show our strategy to prepare gold shell, iron oxide core nanoparticles functionalized with the same ligands. These magnetic composite nanoparticles could be used for mechanical stimulation of the integrin receptors via application of an external magnetic field.

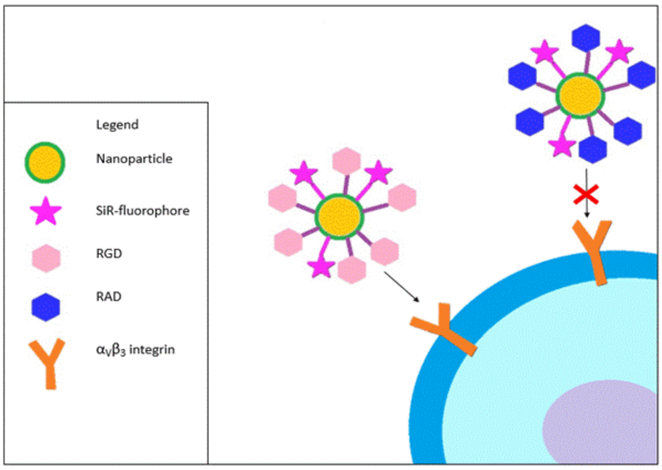

Figure 1: Scheme of the interaction of functionalized nanoparticles with a neuron.

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OR36

Synthesis and biological evaluation of 1,2,4-oxadiazole salts and derived functional materials

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The worldwide rise in antibacterial resistance makes common antibiotics and standard procedures ineffective, providing a significant challenge to contemporary medicine. [1] This phenomenon is not confined to certain clinical environments; rather, it is a systemic issue with implications in surgery, oncology, and the implantation of medical devices. [2] For this purpose, drawing inspiration from a previously published study, [3] a variety of new 1,2,4-oxadiazole pyridinium salts have been synthesized and characterized.

Initially, 37 compounds were tested in vitro against Gram-positive S.aureus and Gram-negative E.coli standard strains via dilution and minimal inhibition concentration (MIC) assay. Subsequently, the 5 most active salts were tested against multidrug resistant strains (K.pneumoniae, E.coli, S.aureus, S.haemolitycus and E.faecium). In addition, their cytotoxicity, hemolytic activity, and selectivity index have been evaluated. After the incorporation into PVC films and glycerol gels, disk diffusion tests and diffusion in aqueous solution have been performed, demonstrating sustained antibacterial activity (i.e. zone of inhibition from 8 to 17 mm). The current study represents an initial step towards the development of possible antibacterial coatings for medical implants.

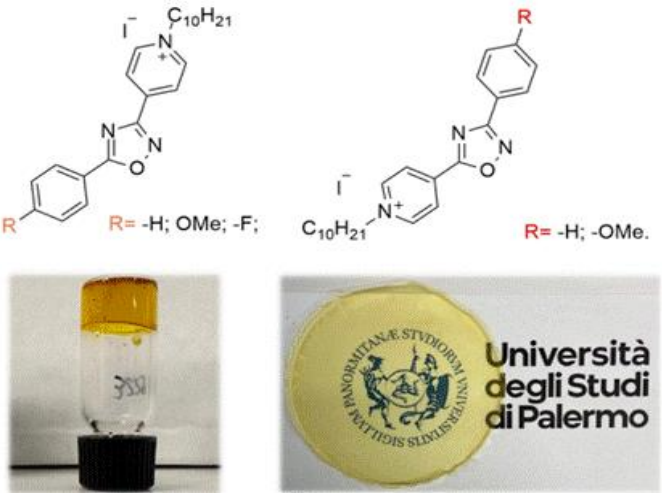

Figure 1: General structures of antibacterial salts, example of derived glycerol-based gel (left) and PVC film (right).

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OR37

Overcoming cancer therapy resistance: the role of arginase inhibitors

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The overexpression of two isoforms of arginase (ARG), ARG1 and ARG2, contributes to the development of several diseases, including cancer. To clarify the specific roles of ARG1 and ARG2 without disrupting their physiological functions, it is essential to develop selective and effective ARG inhibitors with low toxicity and an appropriate pharmacokinetic profile. A promising medicinal chemistry strategy that could be useful in this context is molecular hybridization. This approach could exploit the distinct subcellular localization of the two isoforms to enhance specificity for ARG1 and ARG2, potentially leading to improved therapeutic outcomes, especially in cancers such as gastric cancer, where ARG's hyperactivity has not yet been fully elucidated.

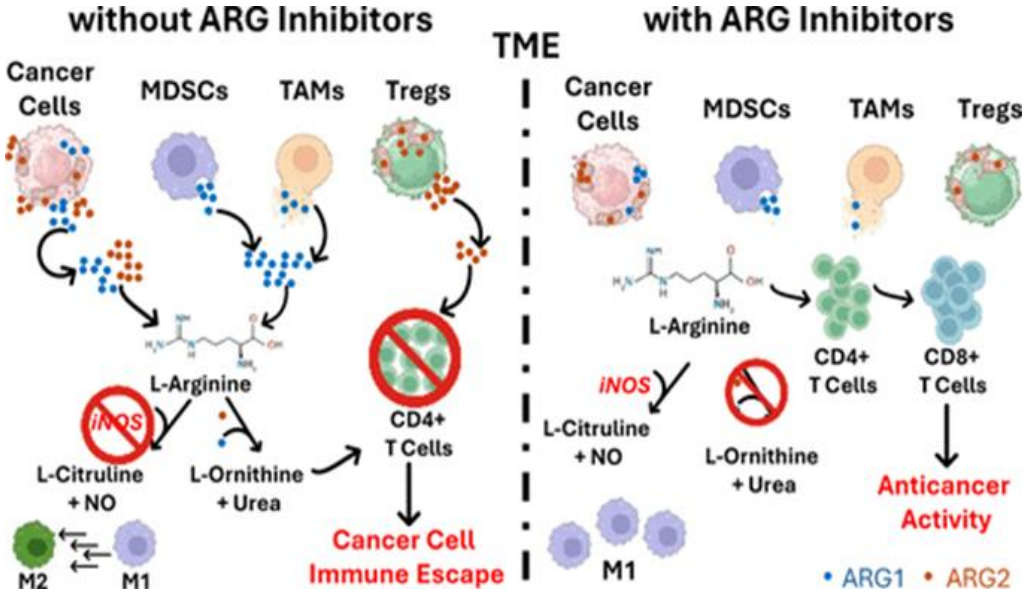

Figure 1: Mechanism of action of ARG inhibitors.

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OR38

New insights into anti-inflammatory biased FPR2 agonism by ureidopropanamide derivatives

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Neurodegenerative diseases such as Alzheimer's and Parkinson's diseases involve the formation of protein aggregates, which activate microglial cells towards a pro-inflammatory phenotype. This phenomenon aggravates tissue damage further via oxidative stress. Thus, the activated microglia could offer us a target to alter disease progression and outcome [1]. G-Protein Coupled Receptor Formyl Peptide Receptor 2 (FPR2) is a Damage Associated Molecular Pattern (DAMP) receptor expressed in microglia, whose DAMP-mediated activation leads to pro-inflammatory signaling. In Alzheimer's Disease, FPR2 is thought to mediate the inflammatory effects of amyloid beta peptides. At the same time, Specialized Pro-Resolving Mediators (SPMs), such as Lipoxin A4 (LXA4), can bind FPR2, yet mediating opposite, anti-inflammatory effects, delineating a complex model of FPR2 pharmacology in which its activation bias depends on the chemical structure of each ligand [1-2]. The structural determinants of biased FPR2 activation are yet to be elucidated. As a first step in this direction, we have leveraged our library of selective ureidopropanamide FPR2 agonists [3]. A few of these compounds had previously been tested for Ca^{2+} mobilization, β-arrestin recruitment, and phosphorylation of ERK1/2 and Akt, showing that structure variations could affect all these pathways. We have thus developed an assay panel to conduct a wide-range screening on ureidopropanamide-based FPR2 agonists. The data from the screening has provided us with valuable insights into the structure-activity relationships of ureidopropanamide derivatives in the context of pro-resolving FPR2-biased agonism.

This work was supported by #NEXTGENERATIONEU (NGEU) and funded by the Ministry of University and Research (MUR), National Recovery and Resilience Plan (NRRP), project MNESYS (PE0000006)—A Multiscale integrated approach to the study of the nervous system in health and disease (DN. 1553 11.10.2022) and by the University of Bari Aldo Moro Call ERC Seeds, Project RENEW-FPR2 (2023-UNBACLE-0245444) — Resolving Neuroinflammation With FPR2 Biased Agonism (DR. 548 15.02.2024), and Project NextGeneration EU_PNRR_M4.C2 Investimento 1.1_PRIN P20227TATA

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OR39

Uncovering a mutation-independent therapeutic strategy against Inherited Retinal Diseases: development of class I HDAC/LSD1 hybrid inhibitors

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Among genetic retinal disorders, retinitis pigmentosa (RP) is characterized by degeneration of rod photoreceptors caused by a large number of diverse mutations, most of them acting through different pathways to which epigenetic targets also contribute [1]. The eraser enzymes lysine demethylase 1 (LSD1) and histone deacetylase 1 (HDAC1) play major roles in the development of rod photoreceptors and their inhibitors were shown to block inherited rod degeneration, preserving vision, and contributing to a general anti-inflammatory profile at retinal level [2]. In this work, we proposed the development of poly-pharmacological agents targeting class I HDAC/LSD1 enzymes with the aim of treating *rd10* mice model of RP. The new small library of compounds is typified by hybrid **(±)-3d** which showed IC_{50} values of 1702, 842 and 358 nM against HDAC1, HDAC2 and HDAC3 respectively, while inhibiting LSD1 with an IC_{50} value of 1074 nM. When tested on hydrogen peroxide-stressed ARPE-19 and 661W retinal cells at the concentration of 10 µM, **(±)-3d** showed a promising antioxidant profile, increasing the cellular levels of acetylated and methylated histone H3 and was selected for further studies also in light of its calculated IH-L. In *rd10* mice RP model, a single intravitreal injection of **(±)-3d**, at the same concentration used in cells, enhanced photoreceptor survival, downregulated retinal expression of the inflammatory genes GFAP, Ccl2 and Ccl12 and effectively preserved the retinal pigment epithelium barrier. Furthermore, **(±)-3d** promoted acetylation and methylation of histone H3, thus confirming the engagement of both class I HDAC and LSD1.

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OR40

Design and development of NPs based on thiolated derivative of Hydroxypropyl-β-Cyclodextrin (HPβCD-SH) for improving ocular delivery of lipophilic drugs

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The effective delivery of drugs to the posterior segment of the eye remains a major challenge in ocular pharmacology. The aim of this study is to develop and characterize nanoparticles based on a thiolated derivative of hydroxypropyl-β-cyclodextrin (HPβCD-SH) for improving the ocular delivery of corticosteroid drugs such as Dexamethasone (DEX), Triamcinolone (TRI), and Triamcinolone Acetonide (TRI ac). The thiolated cyclodextrin was synthesized via chemical modification of HPβCD using thiourea. The degree of substitution (DS) of thiol groups was found to be 0.44 through ^{1}H-NMR analysis, while Ellman's assay was employed to determine the thiol group content and confirm structural integrity [1]. The diameter distribution of the spontaneous nanoaggregates formed by the thiolated derivative, as determined by NanoSight measurements, was found to be 123.3 ± 4.7 nm, with a narrow size distribution and high stability over time. Inclusion complex formation between both the unmodified and thiolated cyclodextrins and the selected drugs was investigated using the Higuchi–Connors method to assess binding capacity and complex stability. In all cases, an increase in the association constant was observed when the thiolated derivative was used. Furthermore, the thiolated cyclodextrin was able to solubilize a higher amount of all three drugs compared to the non-thiolated form (2x for DEX and TRI, 10× for TRIac). Permeation studies were performed using Franz diffusion cells equipped with 3.5 kDa semi-permeable membranes to evaluate drug diffusion from the particles. Based on complexation efficiency and permeation profiles, the 1% HPβCD-SH formulation was identified as the most promising.

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OR41

Light-Dependent Modulation of Bacterial Adhesion as a Novel Antibiofilm Strategy

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Antimicrobial resistance (AMR) represents an escalating global health concern, especially in hospital-acquired infections. A key factor in the persistence and spread of AMR is biofilm formation, able to create a protective environment that enhances microbial survival and promotes horizontal gene transfer. Central to this process are bacterial adhesion proteins, which mediate interactions between microbial cells and surfaces, supporting the growth of resistant communities. These proteins have thus become attractive targets for novel anti-AMR strategies. Among them, lectin LecB, a virulence factor located on the outer membrane of *Pseudomonas aeruginosa*, has gained increasing interest due to its role in pathogenicity as well as its strong carbohydrate-binding ability, interacting with both the bacterial membrane and the biofilm matrix [1]. In this context, this research project aims at developing innovative photoswitchable ligands that enable light-dependent modulation of LecB activity, allowing for precise, minimally invasive therapeutic interventions, and thus overcoming the limitation of conventional bacterial cell adhesion modulators [2]. Based on an initial photoswitchable hit compound designed in our lab, we launched a computationally guided hit expansion to identify new ligands characterized by improved affinity in the *cis*-enriched form, with the final goal of assessing their light-dependent antibiofilm properties. The design, synthesis, photochemical behavior, and preliminary biological profile of the compounds under study will be presented and discussed.

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OR42

New CB2 dualsteric ligands for the treatment of multiple sclerosis

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Multiple sclerosis (MS) is a chronic, highly disabling inflammatory disease characterized by demyelination, axonal damage, and progressive neurodegeneration. Among its diverse clinical manifestations, neuropathic pain is one of the most debilitating symptoms, severely impacting patients' quality of life. Current therapeutic approaches, primarily based on immunomodulatory and anti-inflammatory agents, often fail to halt disease progression or adequately manage symptomatology.

Recent findings have highlighted an increased expression of CB2-immunoreactive microglia in MS patients, suggesting that CB2 receptor modulation may offer a promising and safe therapeutic strategy [1].

This study focuses on the design and synthesis of novel dualsteric CB2 modulators able of interacting simultaneously with both the orthosteric and allosteric binding sites of the CB2 receptor. For this purpose, a ligand-based approach was adopted, combining the selective CB2 agonist COR167 with cannabidiol (CBD) or its analogues. Molecular hybridization techniques were employed to generate a series of hybrid compounds with a variety of linkers which differed in length and chemical properties, to optimally connect the two pharmacophores while preserving key receptor interactions (**Figure 1**).

The synthesized compounds were evaluated *in vitro* using the BV2 murine microglial cell line to assess cytotoxicity and anti-inflammatory activity, providing preliminary insights into their potential therapeutic efficacy in the context of MS.

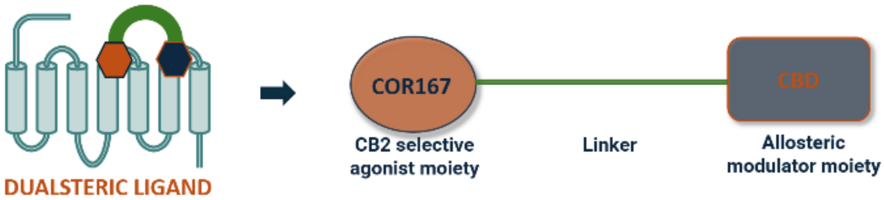

Figure 1: General structure of the dualsteric compounds.

Acknowledgements: European Union - Next Generation EU “Targeting microglia CB2 receptors with novel multisite ligands: a multidisciplinary and translational study for the identification of an innovative multiple sclerosis therapy” (PRIN2022BNSNS2, CUP E53D23012360006).

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OR43

Anodic Decarboxylative Alkylation Reaction of Electron Poor Double Bonds, Enabling a Sustainable and Catalyst-Free Alternative to Minisci-Type Reactions

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Decarboxylative coupling reactions have gained enormous importance in the organic synthesis of pharmaceutically relevant molecules, at particular since the work of Minisci.[1] Current developments deal with new ways of generating radicals by photo- and electrochemical methods, which show a considerable improvement of already known bond formations.[2] Despite the significant advantages of these reactions, one of their major disadvantages is the poor atom economy and the use of expensive metal salts, as well as the contamination of pharmaceutically relevant products with these. Disadvantages that also affect classic Minici-type reactions, in addition to the (over-)stoichometric use of oxidizing agents.[3]

In this work, we aim to address the challenges of previous studies and present a metal-free, direct and complementary alternative to existing methods. We use the direct Kolbe-like decarboxylation of carboxylates to electrochemically generate alkyl radicals, which can then be transferred to electron-poor double bonds while retaining their functionality. Furthermore, by specific cell design, we provide access to reductively sensitive substrates that are often inaccessible by electrochemical or photochemical reactions described in the literature. In this work, we present a wide range of pharmaceutically relevant structural motifs that are being tested as drug candidates or are already in use as active ingredients.

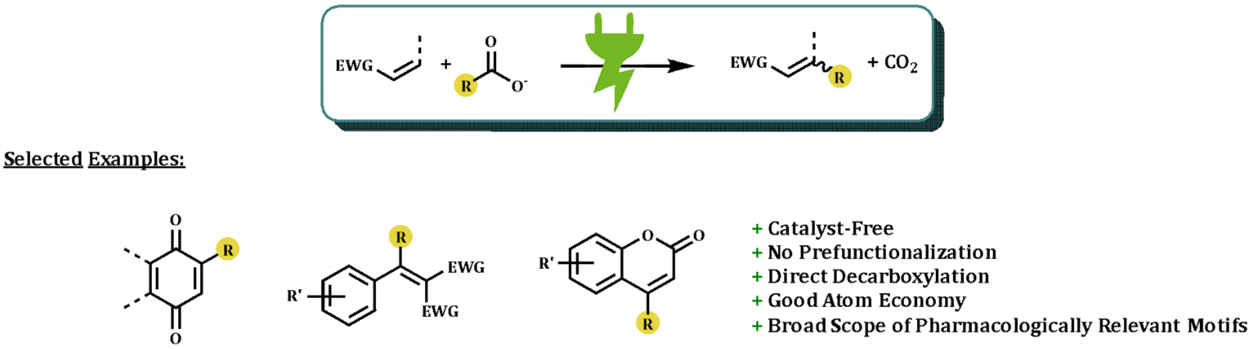

Figure 1: Overview of the proposed decarboxylative coupling reacting as well as selected motives of the reaction scope.

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OR44

Sequential Michael addition/aza-Wacker-type cyclization reaction for the efficient synthesis of fused indolines

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The one-step synthesis of complex *N*-heterocycles, specifically pyridazine–indole motifs, as bioisosteres of β-carbolines, is highly desirable for efficiency and sustainability. Intramolecular aza-Wacker cyclization [1], a type of transition metal-catalyzed amination, efficiently transforms alkene-tethered amines or amides into different saturated *N*-heterocycles (Fig. 1a).

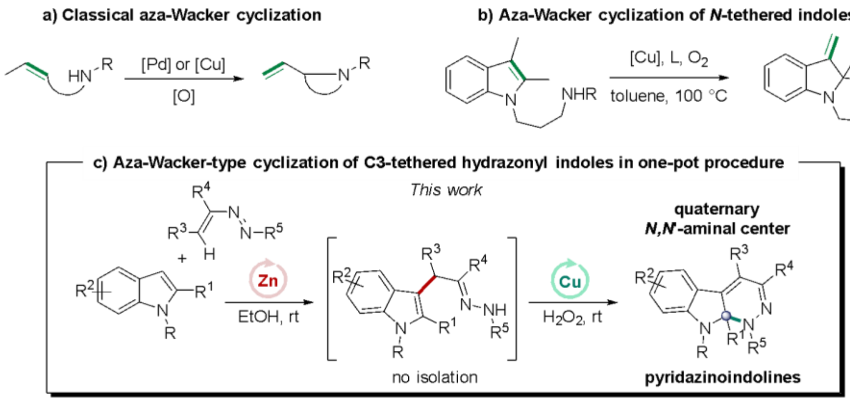

Figure 1: a) Classical aza-Wacker cyclization, b) Aza-Wacker-type cyclization of *N*-tethered indoles, c) Aza-Wacker-type cyclization in our sequential transformation.

Inspired by Shen/Jia work [2] (Fig. 1b), herein we report a one-pot Zn(II)-catalyzed Michael addition/aza-Wacker-type cyclization strategy for synthesizing C-2 quaternary pyridazino[3,4-*b*]indole frameworks. A Cu-catalyzed intramolecular dearomative amination is achieved using H_2O_2 as the sole, mild oxidant at room temperature, avoiding reactive peroxides or high-pressure O_2 (Fig. 1c). This method tolerates a wide range of indole and 1,2-diaza-1,3-diene [3] substrates and provides a safer, greener, and more sustainable route to novel indole–pyridazine scaffolds in good to excellent yields. The resulting products offer structural diversity which could allow for further functionalizations and provide conformational rigidity that may enhance drug-like properties.

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OR45

From life's origin to CO_2 conversion technologies: lessons from alkaline hydrothermal vents

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Oceanic Hydrothermal Vent are geological formations proposed as possible cradles for the emergence of life on our planet. In the Archean era, at the Alkaline Hydrothermal Vent (AHTV) environment, a mineral barrier, composed of iron oxide and hydroxide, iron sulphide, along with Ni, Zn, Co, and Mn ions precipitate creating the vent structure itself. This mineral barrier separates two different environments: the outer acidic with CO_2 and the inner alkaline with H_2, in this situation an electrochemical potential difference is generated across the mineral barrier of the vent structure; this life-like thermodynamic disequilibrium can be dissipated through coupling of CO_2 reduction (CO_2RR) reaction with hydrogen oxidation (HOR), generating the very first organic molecules on our planet. [1]

This fascinating lesson from nature – demonstrating how efficient, low-energy processes, based on abundant and non-toxic materials, can initiate complex chemical syntheses – provides a powerful paradigm for contemporary green chemistry and technological sustainability. Our research focuses on developing "emergence of life inspired materials" for CO_2 conversion, addressing the environmental challenges of the new millennium.

Recently, we proposed a new framework to describe hydrothermal vent behaviour using concepts from electrochemistry: modelling the system as a short-circuited fuel cell, where CO_2RR and HOR occur on distinct mineral "electrodes" that are short-circuited, the process is driven ultimately by the pH gradient between simulated vent fluids and ocean water. Using this model, we detected spontaneous current generation and measure the operating electrochemical potential [2].

Furthermore, we demonstrated that mineral phases such as mackinawite (Fe–S) and violarite (Fe–Ni–S) can catalyse electrochemical CO_2 reduction, producing formic acid, methanol and carbon monoxide at –0.72 V vs RHE, and suggesting that a very low overpotential is needed to reduce CO_2 on these materials. [3] Finally, by combining microfluidics with electrochemistry it was possible to study the formation and growth of the mineral barrier and the establishment of the electrochemical potential difference.

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OR46

Optimization of supercritical CO_2 fluid extraction of lipids from process waste of Organic Municipal Solid Waste treatment plant using Box-Behnken experimental design

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The recovery of energy and matter from wastes is a Circular Economy' key point. In the European Union, the Organic Fraction of Municipal Solid Waste (OFMSW) is made up of organic materials and food wastes, derived from kitchens, markets, parks and represents a potential feedstock that must be valorised in different ways, such as composting and/or the biogas synthesis. In treatment plants, there are several preliminary mechanical process, which also generate process wastes. The Closed-loop management strategy of these wastes can lead to economic and environmental benefits. The chemical composition of this biomass is very heterogeneous and is strongly influenced by waste stream and seasonality: the lipidic content of this complex matrix can be extracted and subsequently chemically converted into biofuels (FAMEs) or biolubricants; FAMEs derived from non edible wastes are classified as "second-generation" biofuels and represent better alternative to non-renewable fossil fuels. In this study, we investigated the supercritical carbon dioxide extraction (sc-CO2 SFE) as Green methodology for lipid recovery, from the plastic bags winnowing waste. Carbon dioxide, above supercritical conditions (73.8 bar and 304.13 K), represent a promising alternative for lipid extraction to the organic solvents (e.g. n-hexane), due to its non-toxic, non-flammability, low cost and very low polarity. After the extraction, the CO2 can be easily removed by expansion at atmospheric pressure, without any contaminations of the extract and the solid residue.

In the preliminary tests, low sc-CO2 SFE yields, compared to the conventional n-hexane Soxhlet extraction (6% wt. lipids vs. lyophilized biomass), were achieved. Therefore, a Box-Behnken design was performed to optimize the SFE conditions of Temperature (303-363 K), Pressure (60-600 Bar), CO2 Flow Rate (4-10 L/min) and Time (30–120 min) to maximize the lipid yields. Model building, experimental results and designs were processed using Minitab® 19.1.1 software. The response Factors were fitted to a second-order regression equation acquired by the Response Surface Methodology (RSM). From the analysis of variance (ANOVA) with 95% confidence level, the model was suitable for the data observed, with quadratic correlation coefficient (r2) up to 90% and the p-value of Lack-of-Fit higher than 0.05. All the linear factors were significant (α>1.45), while in contrast just Pressure*Temperature interaction resulted significant: the most influential factor was the pressure and its square, with up to 80% of model contribution. Positive linear trends were obtained for Temperature and Flow vs. Response, while for the Pressure and Extraction Time, an exponential trend emerged, with a maximum around 470 Bar and 90 min. Optimized parameters to obtain the highest extraction yield were the following: 363 K, 474.5 Bar, 10 L/min and 91.8 min.

OR47

Phytochemical and biological characterisation of red apple pomace extracts obtained using natural deep eutectic solvents and a response surface approach

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In circular economy, food industry waste and by-products gain renewed value by using them to obtain new, promising products, such as functional foods, supplements and others. Coupling these applications to green techniques and solvents minimises the environmental impact of industrial processes. In this regard, natural deep eutectic solvents (NADES) are at the frontier of green extraction solvents [1], having many advantages in terms of compound solubility and environmental and economic perspectives. An interesting kind of food industry by-product is apple pomace (AP), the solid residue of apple fruits after industrial transformations, which contains a higher amount of phenolic compounds than the pulp [2] and, in the case of red varieties, of anthocyanins (such as cyanidine-3-*O*-galactoside or ideain), all compounds well-known for their antioxidant activity, leading to potential applications in different fields. This project aims to optimise the extraction of anthocyanins and other flavonoids from six varieties of red AP using NADES and green technologies. Two green techniques, UAE (ultrasound-assisted extraction) and MAE (microwave-assisted extraction), and NADES mixtures with different component ratios were investigated and compared with traditional extraction solvents and techniques in terms of TAC (total anthocyanin content), antioxidant activities and concentration of bioactive compounds, as assessed by original HPLC-DAD and HPLC-MS methods. MAE extraction coupled to choline chloride: citric acid (2:1) with 50% water gave the best results and underwent additional evaluation, using the RSM (Response Surface Methodology) approach to optimise processing. Solid-to-liquid ratio, temperature and extraction time were used as X variables, while ideain content and Oxygen Radical Absorbance Capacity (ORAC) were selected as Y responses. The optimised conditions thus obtained were applied to produce extracts from all considered apple varieties. Conventional and NADES extracts were assessed for their cytotoxic, anti-inflammatory and antioxidant activities, highlighting the potential applications of red AP.

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OR48

New frontiers in the conversion of fructose to 5-hydroxymethylfurfural: the potential of covalent organic frameworks as catalysts in Deep Eutectic Solvents.

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In recent years, there has been a growing interest in the valorization of lignocellulosic biomass since it could be a valid substitute for oil. Indeed, biomass is a zero-emissions source of materials, it is renewable and available [1]. Among the various value-added chemicals that can be obtained from lignocellulosic biomass, 5-hydroxymethylfurfural (5-HMF) stands out because it can be converted into a range of industrially relevant products, thanks to its several functional groups [2]. Herein, we studied the conversion of fructose to 5-HMF, using sulfonic acid-appended covalent organic frameworks (COFs) as catalysts in cholinium-based deep eutectic solvents (DESs). Covalent organic frameworks (COFs) are porous crystalline polymers constructed from organic building blocks with permanent porosities [3]. We prepared and characterized COFs from 1,3,5-trihydroxy-phloroglucinol with 2,4-diamino-benzenesulfonic acid and with 4,4′-diamino-2,2′-stilbenedisulfonic acid to be used as catalysts for the fructose conversion reaction.

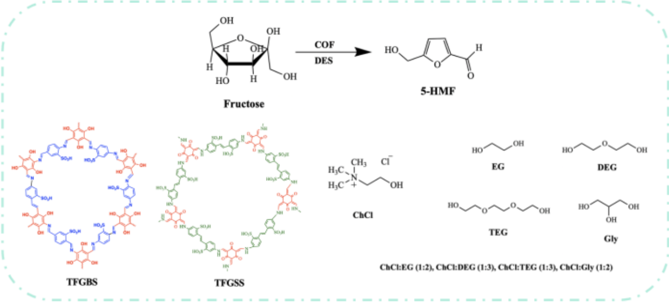

Figure 1: Schematic depiction of reaction, catalysts and solvents.

Both COFs have shown their potential as catalyst for the reaction, leading to obtain high yields in 5-HMF at 120 °C, in particular when we used ChCl:DEG as solvent. Finally, we also explored the recyclability of the catalyst/solvent system.

We thank MUR 20222H43S2 PRIN 2022 - Hybrid Porous Materials for Eco-sustainable Catalytic Organic Processes.

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OR49

Lewis acids *vs* Brønsted acids in the chemical recycling of polylactic acid: a comparison of catalytic efficiency

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Recycling is essential for shifting from a linear economic model to a more sustainable, circular economy. Among the various recycling technologies, the chemical method represents a favourable approach for producing recycled plastics of comparable quality to virgin plastics [1]. Among different polymers, Polylactic acid (PLA) is an excellent example of a bio-based and biodegradable polymer. Under industrial composting conditions, PLA breaks down into only water and carbon dioxide, and its degradation in natural environments is very difficult; therefore, effective recycling methods (especially chemical) are fundamental for PLA. This method allows the recovery of monomers and valuable platform chemicals, preserving both the material's utility and its economic importance. Deep eutectic solvents (DESs) offer a promising pathway to improve the depolymerization process: the acidic nature of DES, whether Lewis or Brønsted, considerably influences reaction mechanisms and results. DES are typically composed of proton donors with quaternary ammonium salts that facilitate depolymerisation via protonation and hydrolysis of ester linkages, often leading to slower depolymerisation and lower product selectivity. To accelerate the depolymerisation process, microwave (MW) irradiation can be employed; in fact, it offers efficient heating compared with conventional methods. The polar molecules in the DES directly interact with microwaves, generating rapid molecular agitation and rotation that leads to productive energy transfer to the reaction medium [2].

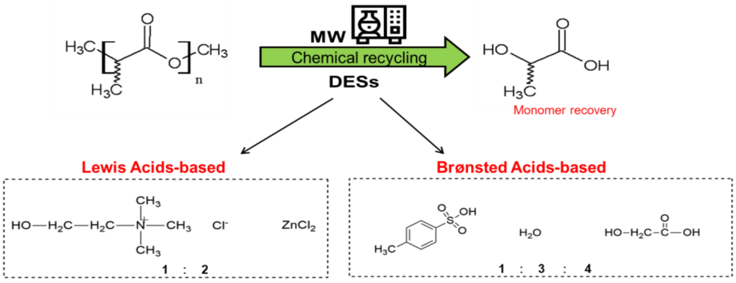

Figure 1: PLA chemical depolymerisation and Lewis acid *vs* Bronsted Acid DESs.

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OR50

Supercritical fluid chromatography to improve the sustainability of methods for lipidomics

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Growing attention is being directed toward the environmental impact of analytical workflows in lipidomics, stimulating the development of greener and innovative methodologies. Currently, this transition is of particular relevance as lipidomics continues to advance in key research areas, including food safety, nutrition, and disease. Conventional chromatographic techniques, such as high-performance liquid chromatography (HPLC), although widely applied, often rely on large volumes of organic solvents that are toxic, costly, and environmentally burdensome.

To address these challenges, this research explored the potential of supercritical fluid chromatography (SFC) as a greener analytical approach for lipid profiling in complex food matrices. Both animal- and plant-derived products were investigated with the dual objective of assessing their nutritional value and ensuring product authenticity and traceability.

This chromatographic technique employs recycled carbon dioxide (CO_2) in its supercritical state as the main component of the mobile phase, combined with minimal amounts of organic modifiers. The unique physicochemical properties of CO_2, such as its low viscosity and high diffusivity, allow for improved chromatographic efficiency and shorter run times. Moreover, compared to conventional HPLC, SFC offers complementary selectivity and a wider range of experimental parameters available for optimization, including the type and concentration of organic modifiers, system back-pressure, and mobile phase density.

The findings of this research highlight the effectiveness of SFC for lipidomic investigations, demonstrating its capacity to deliver robust and reproducible results while minimizing environmental impact. Overall, this technique emerges as a viable and advantageous alternative for lipid profiling, offering clear advantages that align with the principles of green analytical chemistry and paving the way for a more sustainable future in lipidomics.

Acknowledgments: The authors gratefully acknowledge the support from Merck KGaA and Shimadzu Europa.

OR51

An early-stage assessment of lab-scale glycerol carbonate preparation through the LCA methodology

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The scientific community is increasingly directing its research toward more sustainable technological solutions. One of the most emerging issues is the still deep-rooted dependence on fossil resources, which are proving to be inadequate, not only due to their limited and non-renewable nature, but also for the serious environmental, economic, and social consequences associated with their exploitation. In this context, biodiesel production has significantly increased to reduce reliance on traditional fossil fuels, and its market is expected to grow steadily due to rising demand. However, this process results in an oversupply of glycerol, the main byproduct of biodiesel manufacturing, accounting for 10% by mass of the fuel [1]. The conversion of glycerol into glycerol carbonate (GlyC) represents a valuable pathway for its valorization. Notably, GlyC is widely used in various fields, as well as polymer and pharmaceutical production, serving as a chemical intermediate, solvent, and organic electrolyte carrier in supercapacitors. It can be obtained through different pathways, employing direct or indirect sources of carbon dioxide. Glycerol carbonate is mainly produced via transesterification of organic carbonates with glycerol using alkaline catalysts, an efficient process carried out in mild conditions. The direct carbonation of glycerol with CO_2 is also a promising and desirable method to produce glycerol carbonate, due to the need to convert the CO_2 into value-added chemicals, and various catalyst systems such as metal oxides, ionic liquids, and supported solid bases, have been extensively studied for this reaction. The reaction of glycidol with CO_2 is also a worthwhile route for glycerol carbonate production, with recent achievements in efficient synthesis conducted under intensified flow conditions. Finally, glycerol carbonylation with urea is a further effective method to produce glycerol carbonate, where the ammonia generated as a by-product could be recycled to produce urea through the reaction with CO_2, enabling an advantageous process [2]. The aim of this work is to compare the aforementioned synthetic approaches in terms of their environmental impacts, referring to lab-scale process to obtain 100 g of GlyC as the functional unit of the study. Environmental impacts will be calculated using the ReCiPe 2016 method and expressed in scores related to relevant impact categories. The hotspots of the processes in their whole cradle-to-gate route will be also identified and the total primary energy consumption will be assessed using the Cumulative Energy Demand method.

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OR52

From renewable monomers to functional elastomers: sequential organocatalytic strategies for sustainable TPEs

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Thermoplastic elastomers (TPEs) are a class of block copolymers characterized by a microphase-separated morphology, in which flexible amorphous segments impart elasticity while semicrystalline or glassy domains provide physical crosslinks. This dual organization enables rubber-like mechanical properties combined with melt processability. Conventional examples such as styrene–butadiene–styrene (SBS) have stimulated the development of sustainable analogues derived from biodegradable and renewable resources. Among these, aliphatic polyesters obtained through the ring-opening polymerization (ROP) of cyclic esters, including lactones and lactide, are particularly attractive [1]. However, toxicity issues associated with metal-based catalysts such as $Sn(Oct)_2$ have prompted the exploration of environmentally benign catalytic alternatives [2].

Hydrogen-bonding organocatalysts - especially bisurea derivatives and their ureate anions have proven highly effective, offering controlled ROP even for sterically hindered or low reactivity monomers [3].

In this work, we employed ureate anions to implement a sequential two-step polymerization strategy under mild, room-temperature conditions and in short reaction times. In the first step, various lactones were copolymerized to produce an amorphous soft segment, where combinations such as δ-hexalactone and ε-caprolactone effectively suppressed crystallinity. In the second step, lactide was polymerized to form a semicrystalline hard segment, yielding the biphasic morphology typical of thermoplastic elastomers. Overall, this approach demonstrates the potential of organocatalytic ROP to access fully renewable, structurally tunable polyester-based TPEs, paving the way toward sustainable alternatives to conventional petrochemical elastomers.

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OR53

Assessing cellular toxicity through the use of portable electrochemical strips

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Nitric oxide (NO) is a key mediator of physiological and pathological processes, and its stable metabolite nitrite is widely recognized as a reliable indicator of NO production [1]. Conventional analysis by the Griess assay, although well established, requires multiple reagents, extended handling, and spectrophotometric instrumentation. We present a simple and low-cost electrochemical platform based on screen-printed electrodes on a flexible polyester film for the direct determination of nitrite in the supernatants of lipopolysaccharide (LPS)-stimulated macrophages. The device achieves micromolar sensitivity, with a detection limit of approximately 1.5 μM, and its measurements closely correlate with the Griess method (80–136%) without requiring any electrode modification. Beyond detection, the sensor was successfully applied to monitor the anti-inflammatory response to three mechanistically distinct drugs (erucin, naproxen, and deflazacort), demonstrating its suitability for assessing both cellular toxicity and therapeutic effects. Combining portability, low cost, and operational simplicity, this platform represents a practical alternative to conventional assays for nitrite monitoring and the investigation of NO-mediated biological processes.

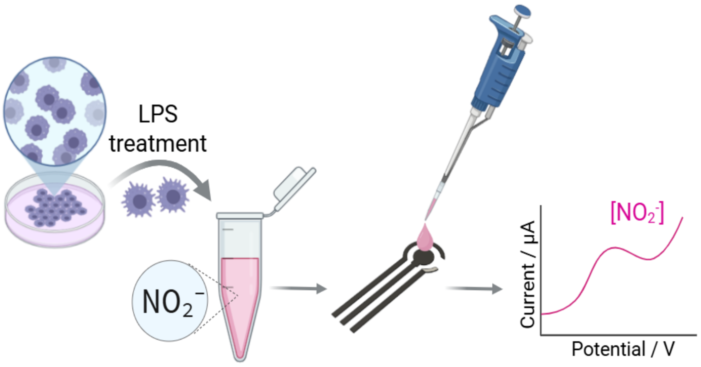

Figure 1: Nitrite (NO_2^-) produced by LPS-stimulated macrophages is quantified from culture supernatants using a screen-printed electrochemical sensor and differential pulse voltammetry (DPV).

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OR54

Enhanced co-reactant electrochemiluminescence for bead-based immunoassays

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Electrochemiluminescence (ECL) is a powerful bioanalytical technique due to its high signal-to-noise ratio and low detection limits [1]. By exploiting the bead-based immunoassay technology, Roche Diagnostic started to produce automated analyzers, making ECL viable for clinical diagnosis [2-3]. The system employs biotinylated and dye-functionalized antibodies that specifically recognize a target antigen. When the analyte is present the classical sandwich assay is formed and the generated ECL signal is proportional to the analyte concentration. Commercialized ECL-based immunoassays typically exploit the heterogeneous co-reactant mechanism between tris(2,2’-bipyridine)ruthenium(II) ($[Ru(bpy)_3]^{2+}$) and tri-*n*-propylamine (TPrA) as luminophore and co-reactant, respectively. The beads-based immunoassay is based on the heterogeneous co-reactant ECL mechanism where the Ru(II) complexes are not directly oxidized. Instead, to produce the emitting $[Ru(bpy)_3]^{2+*}$, the $[Ru(bpy)_3]^{2+}$ labels are reduced by $TPrA^{\bullet}$ and then excited by the electrogenerated $TPrA^{\bullet+}$. In commercial bead-based immunoassays, the enhancement of the ECL signal is achieved by modifying the system (i.e., employment of novel luminophores with higher quantum yield compared to $[Ru(bpy)_3]^{2+}$ or introduction of nanomaterials), but there is a lack of direct approaches [3]. Being the ECL response determined by the radical intermediates’ lifetimes and diffusion distances, a mechanism insight is key to achieving a greater emission. We investigate the reaction mechanism underlying the modulation of the ECL signal of $[Ru(bpy)_3]^{2+}$ labels anchored to magnetic beads. Specifically, we analyze the emission of Ru(II) labels on single beads through a combination of ECL imaging techniques, exploring the interaction with persulfate.

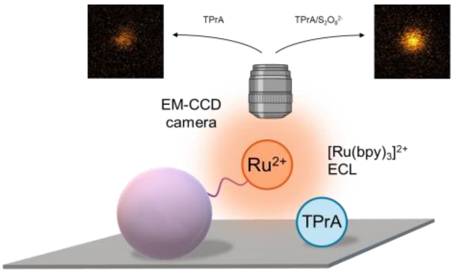

Figure 1: $[Ru(bpy)_3]^{2+}$-labeled magnetic bead under the ECL microscope.

This work was supported by ECLectic project that has received funding from the European Union's MSCA Doctoral network Horizon Europe programme Grant Agreement Number 101119951.

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OR55

Decentralized electroanalysis and chemometrics: a potent merging for new analytical applications

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Electrochemical sensors are increasingly recognized as powerful tools for decentralized and cost-effective analysis, offering portability, rapid response, and low cost. Nevertheless, their practical applicability is often challenged by signal overlap and matrix interferences. Chemometrics provides an effective solution to these limitations, enabling data-driven optimization, classification, and improved analytical performance[1].

In this work, we present the integration of electroanalysis with chemometric approaches as a promising strategy for innovative analytical applications. As a case study, a homemade polyester screen-printed electrode was employed for the electrochemical detection of cannabidiol (CBD) in Cannabis sativa extracts. The sensor exhibited good reproducibility and sensitivity, and its performance was benchmarked against liquid chromatography–tandem mass spectrometry (LC-MS/MS).

Principal component analysis (PCA)[2] was then applied to resolve the electrochemical overlap between CBD and tetrahydrocannabinol (THC), allowing the clustering of real samples including *hashish, marijuana,* and *C. sativa* extracts. This combined strategy not only distinguished CBD-rich from THC-dominant products but also demonstrated the potential of merging sensors and chemometrics for quality control in complex matrices.

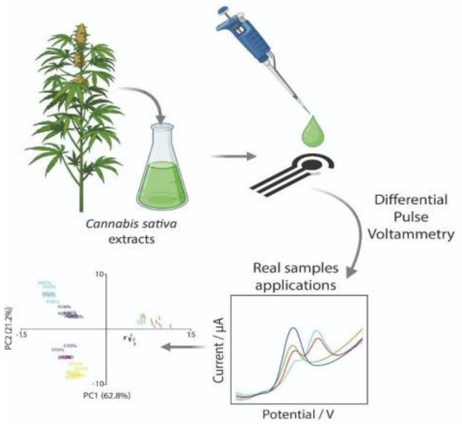

Figure 1: Schematic worflow.

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OR56

Synthesis of bispidine-based fluorinated chemosensors for selective metal ion recognition

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Nuclear magnetic resonance (NMR) is a powerful analytical technique for studying molecular organization and atomic-level structure. However, its interpretation can be challenging due to the complexity of spectra caused by signal overlap and low sensitivity [1]. To address this issue, chemosensing systems use specific molecular interactions to generate simplified, distinguishable signals, allowing simultaneous detection of multiple species [2].

The use of ^{19}F-labeled molecular probes for the coordination of analytes allows the generation of unique, distinguishable ^{19}F NMR signals with minimal background interference (Figure 1) [1]. Among these, metal-chelating fluorinated probes represent an advanced class of F-probes designed for dual-mode imaging or stimuli-responsive theranostics. These hybrid probes combine the molecular specificity of ^{19}F NMR with the paramagnetic properties of metals like Gd^{3+}, Mn^{2+}, Fe^{3+}, or Cu^{2+}, to enhance both imaging and therapeutic effects [3].

In this work, bispidine, a heterocyclic compound consisting of two fused piperidine rings, was selected as a scaffold for metal chelation thanks to its rigid framework, conformational adaptability and multiple nitrogen donor atoms. Mannich reaction allows selective introduction of ^{19}F-labelled probes (such as F, CF_3 and OCF_3) and additional nitrogen atoms to enhance coordination. Two types of scaffolds were prepared: bidentate bispidines via one-pot Mannich reaction and tetradentate bispidines via a multi-step Mannich reaction. These compounds were fully characterized and tested to evaluate their ability to selectively recognize different metal cations.

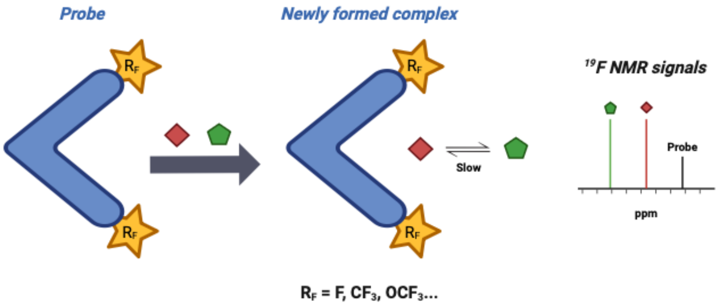

Figure 1: Detection of analytes via ^{19}F NMR chemical shift

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OR57

From gadolinium(III) to iron(III): coordination polymers for T_1-MRI and photothermal therapy

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Coordination polymer-based systems, particularly those incorporating Fe(III), are gaining attention for biomedical imaging due to their tunable morphology, biocompatibility, and potential for surface functionalization[1]. Thanks to its five unpaired electrons, Fe(III) represents a safer and valuable alternative to Gd(III) for MRI, especially for T_1-weighted imaging. While low molecular weight Fe(III) chelates have been explored, the development of Fe(III)-based nanostructures as efficient T_1 MRI contrast agents remains less investigated. In this study, we report the synthesis and characterization of Fe(III)/gallic acid coordination nanoparticles coated with low molecular weight polyethylene glycol (PEG), designed to enhance second-sphere water interactions with Fe(III) ions exposed on the nanoparticle surface and increase longitudinal relaxivity at clinical magnetic fields (1.5 – 3.0 T)[2]. This strategy proved to be effective, as PEG/Fe(III)-GA nanoparticles exhibited relaxivity values per Fe(III) ion exceeding those of the PVP-coated analogues by more than 150% at 3 T and 298 K. Moreover, these nanoparticles demonstrated excellent performance in photothermal therapy (PTT), highlighting their potential for cancer theranostics. Furthermore, their aqueous suspensions showed prolonged colloidal stability, high biocompatibility, and satisfactory *in vivo* MRI contrast, even at low administered doses.

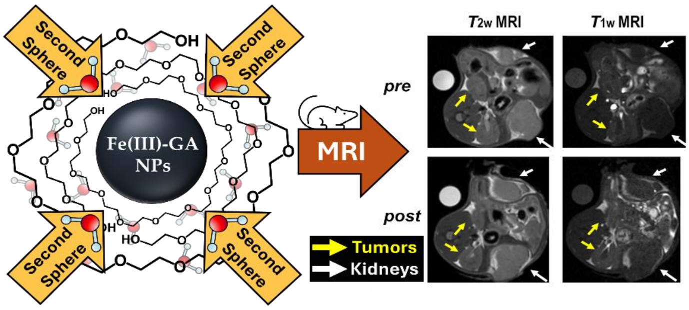

***Figure 1**: Schematic representation of Fe-GA nanoparticles coated with PEG polymer, and MRI images of a mouse model before and after injection of the nanoparticle suspension.*

Acknowledgements: This work was supported by Unione europea- Next Generation EU, Missione 4 Componente 2 CUP D53D23016730001

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OR58

Mesoporous bioactive glasses as multifunctional materials for biomedical applications

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The discovery of 45S5 Bioglass® in 1969 marked a milestone in biomaterials research. Since then, bioactive glasses have been widely explored for tissue repair and drug delivery [1]. However, surgical implantation often triggers inflammation and oxidative stress due to reactive oxygen species (ROS), which can delay healing. Materials capable of neutralizing ROS are therefore highly desirable [1].

Mesoporous bioactive glasses (MBGs) are particularly effective as drug delivery systems due to their high surface area and pore volume. Their functionality can be enhanced by incorporating therapeutic inorganic ions (TIIs), which promote angiogenesis, osteogenesis, cementogenesis, and antibacterial activity.

Professor Lusvardi's research group has focused on the use of cerium as TII, which provides antioxidant, antitumoral, antiemetic, and bacteriostatic effects. Its antioxidant activity stems from the coexistence of two oxidation states (Ce^{3+}/Ce^{4+}), enabling the material to counteract oxidative stress [2]. Our recent studies [3] have explored dual-ion doping (Ce/Cu, Ce/Ag, Ce/Mg, Ce/Sr) and functionalization with polyphenols or drugs (ibuprofen, paracetamol, gentamicin) to expand therapeutic potential. The aim is to develop MBGs co-doped with TIIs and functionalized with biomolecules, while preserving bioactivity and creating multifunctional materials for advanced biomedical applications.

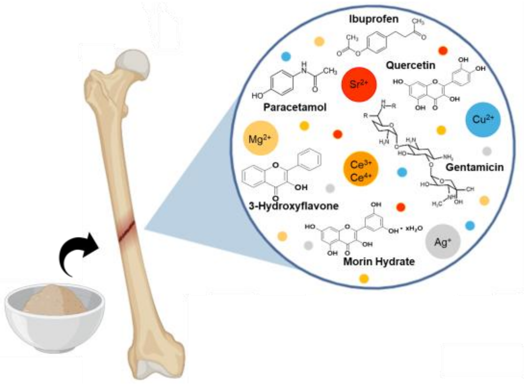

Figure 1: Bone treated with ion-doped MBG loaded with drugs and polyphenols.

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OR59

Albumin oxidation alters protein binding capability to Amyloid-β peptide

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Human serum albumin (HSA) is the most abundant protein in both plasma and cerebrospinal fluid (CSF) and is involved in different functions, among which the maintenance of the redox state and the possibility to bind many ligands [1]. Amyloid beta (Aβ) represents one the main binding partner for HSA, as the latter can transport Aβ from the CSF to the blood and inhibit its aggregation [2]. However, oxidative stress conditions, as those encountered in pathologies such as Alzheimer's Disease (AD), lead to protein damages and induce conformational changes that can alter HSA binding capability. Interesting, a higher amount of oxidised HSA was found in the CSF of AD patients [3]. These evidences indicate a possible involvement of oxidised and misfolded HSA in AD development and progression. However, to the best of our knowledge, no studies are reported in the literature about the interaction between Aβ and oxidised HSA.

In this work, a systematic approach was applied to study the effect of oxidative stress on HSA conformation when the same number of equivalents of two different oxidant agents is employed. A recombinant form of HSA isolated from transgenic *Oryza Sativa* (OrsHSA) was used for this purpose. Oxidation was performed by Chloramine T (CT) and Metal Catalysed Oxidation (MCO). Conformational changes characterization was carried out by absorption, fluorescence, 8-Anilino-1-naphthalenesulfonic acid (ANS) binding assay. Differences in the oligomeric distribution were investigated by FPLC and SDS-PAGE. Finally, measurements of the Diffusion Coefficient (D) were performed through a new Surface Plasmon Resonance (SPR) based approach, known as *D*-SPR. Results obtained show that the two systems lead to different oxidative damages on HSA. In particular, CT mainly alters OrsHSA conformation whereas MCO also affect its oligomerization/fragmentation pattern. In addition, the interaction between $A\beta_{1-40}$ and wild type/oxidised OrsHSA was investigated by SPR in order to detect any change in OrsHSA binding capability to $A\beta_{1-40}$ upon oxidation. Results show a decrease in the affinity of oxidised OrsHSA for $A\beta_{1-40}$.

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OR60

From micro to nanospheres for smart coatings development

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Smart coatings have recently emerged as an advanced and versatile class of materials. Due to their ability to interact with the environment and to respond to external stimuli, they can provide a wide range of functionalities including self-healing, antimicrobial activity, anti-corrosion, controlled release, and self-cleaning [1]. One effective strategy to develop such intelligent surfaces is the incorporation of pre-formed functional nanoparticles, typically through techniques like spin coating, to form nanocomposite coatings.

Expanding on this idea, our attention has been focused on the introduction of polymeric nanospheres, which offer various advantages such as reduced dimensions, surface tunability, and encapsulation potential. As model system, polymeric microspheres were developed through a simple and fast microfluidic technique, involving an infusion pump. By drop-casting a solution of epoxy-dodecylamine polymer into a continuous phase [2], spheres with a diameter of 10–80 µm were successfully formed (Figure 1a). One notable advantage of this protocol is the possibility to readily modify both the sphere surface and inner content by dispersing additives, small molecules or carbon nanostructures in the polymer or in the water solution, respectively.

Once the microsphere fabrication procedure was optimized, we moved on to the preparation of polymeric nanospheres, by using an ultrasonic tip. This approach enabled the formation of nanospheres with significantly reduced diameters (200-250 nm, Figure 1b) and improved stability, suitable for the application in advanced coatings formation. Their integration enhances the physical and chemical properties of the coverings, allowing their use in various fields such as drug delivery, engineering, and electronics.

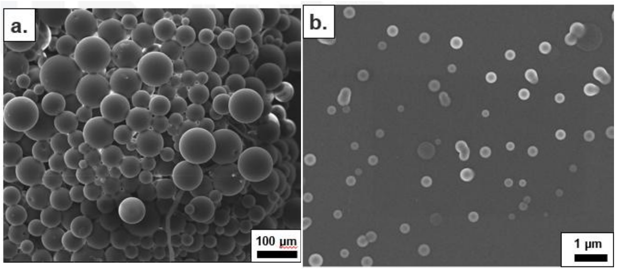

Figure 1: a. SEM images of polymeric microspheres. b. SEM images of polymeric nanospheres.

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OR61

Schiff Base/MoS_2-Modified Electrodes for Sensitive Detection of Lead ions

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Environmental concerns over heavy metals (HMs), particularly Pb^{2+}, are growing due to their toxicity, persistence, and tendency to bioaccumulate in the human body, contributing to cancer and infections across multiple organ systems [1,2]. Traditional detection methods, such as atomic absorption spectroscopy (AAS) and inductively coupled plasma mass spectrometry (ICP-MS), provide high sensitivity and precision but are costly, require extensive sample preparation, and are not suitable for rapid, on-site monitoring. Screen-printed carbon electrodes (SPCEs) offer a cost-effective platform for real-time HMs detection [3]. In this study, SPCEs were functionalized with MoS_2 nanosheets covalently linked to two novel Schiff bases (SB1 and SB2) via monochloroacetic acid (MCA). The resulting MoS_2-SB1 and MoS_2-SB2 sensors were tested for Pb^{2+} detection using square wave anodic stripping voltammetry (SWASV). Both sensors showed enhanced electrochemical responses compared to bare electrodes, with MoS_2-SB2 exhibiting superior sensitivity (LOD: 0.267 μM, linear range: 1–5 μM) and high selectivity in real water samples. These results highlight the potential of MoS_2-SB2/SPCEs as efficient sensors for lead monitoring.

Figure 1: *MoS_2-SBs for Pb^{2+} electrochemical detection*

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OR62

Chemo-enzymatic synthesis of stilbenoid metabolites and derivatives as potential antimicrobial agents

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Stilbenoids are a class of non-flavonoid polyphenols characterized by two aromatic rings connected by an ethylene bridge. Among them, resveratrol is the most extensively studied, abundant in grapes and wine, as well as in residues and byproducts derived from their processing [1]. Although it is scarcely detectable in plasma and tissues upon oral consumption, various and significant bioactivities *in vivo* have been reported, suggesting a crucial role of its metabolites [2]. Among stilbenoids, pterostilbene and deoxyrhapontigenin have also attracted scientific interest due to their potential health benefits. A versatile synthetic approach has been developed to attain a collection of stilbenoid metabolites and derivatives in sufficient amount for biological evaluation and systematic SAR studies. The collection was designed combining modifications associated with phase I metabolism (i.e. reduction of the double bond, dehydroxylation and methylation of the phenolic hydroxyl groups). The synthesized compounds have been tested for their antimicrobial properties against a representative panel of Gram-positive and Gram-negative bacteria and relevant phytopathogenic fungi (*P. oryzae*, *B. cinerea*, and *F. culmorum*). The obtained results showed moderate to good activity against the selected bacterial strains with MICs of 8-128 μg/mL. Notably, several compounds showed remarkable antifungal potential, with over 50% inhibition of the mycelial growth at 200 μM. Moreover, most compounds effectively inhibited spore germination and appressorium formation (a specialized dome-shaped infection structure), even at 50 μM.

This investigation is partially supported by National Recovery and Resilience Plan (NRRP), Mission4 Component 2 Investment 1.3 -Call for tender No. 341 of 15/03/2022 of Italian Ministry of University and Research funded by the European Union–NextGenerationEU, in the frame of the project: Research and innovation network on food and nutrition Sustainability, Safety and Security (ON Foods)

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OR63

Selective and sensitive vapochromic detection of pyridine vapors using smartphone-assisted RGB color analysis

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Pyridine (Py) is a volatile aromatic amine widely used in industries, especially for synthetic processes. Inhalation, ingestion, or skin absorption of this substance can lead to acute symptoms of intoxication [1]. Its release into the environment can therefore represent a significant risk to environmental safety and human health. For these reasons, the selective and sensitive detection of Py vapors using simple detection methods is highly desirable.

To this end, a Lewis acidic Zn(salen)-type complex having vapochromic properties [2] was chosen for the development of paper-based sensors (PBSs), as potential chemosensor for the vapor-phase detection of this volatile amine.

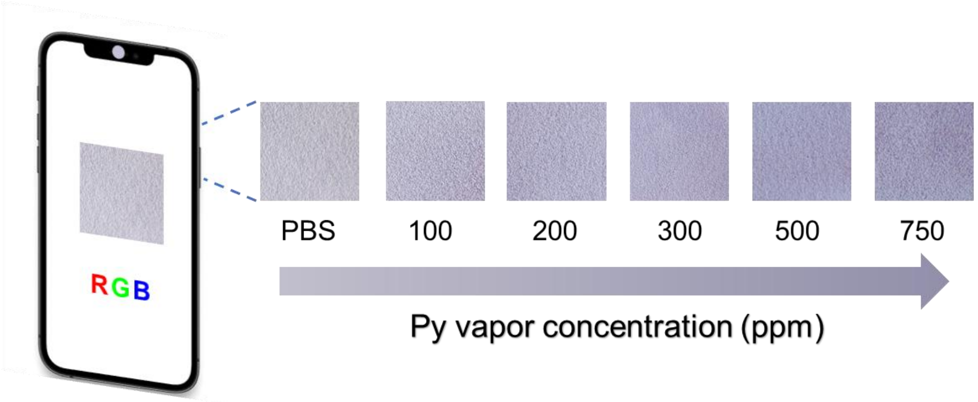

Figure 1: RGB color analysis of PBS before and after exposure to Py vapors.

Using reflectance spectra and smartphone-assisted RGB color analysis, a selective and sensitive response of PBSs towards Py vapors was obtained, compared to other investigated VOCs, independent of the lighting conditions and the smartphone used. Furthermore, PBSs exhibit a linear dynamic response in a range of Py vapor concentrations up to 750 ppm (Figure 1) and a calculated LOD (36 ppm) lower than the NIOSH established IDLH value for Py (1000 ppm).

In summary, vapochromic PBSs based on a Zn(salen)-type complex, in combination with RGB color analysis, allow a simple and quantitative on-site detection of Py vapors.

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OR64

Comprehensive LC×LC for food analysis: principles, strategies, and recent developments

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Comprehensive two-dimensional liquid chromatography (LC×LC) is an advanced separation technique that combines two liquid chromatography systems with distinct selectivities, offering a powerful alternative to conventional one-dimensional LC.

By significantly enhancing peak capacity and resolving power, LC×LC is particularly well-suited for the analysis of highly complex matrices. This contribution provides a detailed overview of the fundamental principles and methodological considerations underlying LC×LC, with a focus on the rational selection of column combinations, modulation strategies, and optimization of chromatographic conditions.

Emphasis is placed on the practical implementation of comprehensive LC×LC workflows for the analysis of food matrices, addressing critical aspects such as system compatibility, modulation efficiency, and data handling. Within the field of food analysis which encompasses the assessment of composition, quality, safety, traceability, and nutritional value LC×LC demonstrates clear analytical advantages.

The technique enables the resolution of co-eluting species, reduces the impact of matrix effects and improves quantitative performance, particularly when coupled with mass spectrometry.

Recent applications focused on the characterization of polyphenolic compounds highlight the potential of LC×LC as a green analytical strategy. In particular, the possibility to operate with simplified sample preparation protocols and more efficient analyte separation paves the way for more sustainable workflows in line with current trends in eco-conscious method development.

OR65

Removal of lithium in aqueous solution using spent halloysite-based catalysts and its electrochemical detection using screen-printed carbon electrodes modified with $LiMn_2O_4$

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This study aims to comply with the circular economy principles, focusing on the reuse and recycle of waste materials from catalytic processes in a sustainability way, i.e., the removal of potentially toxic metal cations from aqueous solutions, and achieving an accurate alternative strategy for metal detection. In particular, the recycling of the nickel-based catalysts, i.e., spent aluminosilicate nanotubular clay supports (e.g., halloysite (HNT)), previously developed and used for dry reforming of methane (DRM) [1], is proposed here for the removal of lithium (Li^+), one of the most important metals in the energy industry for use in energy storage and in the transition to renewable energy due to its reactivity. However, exposure to excessive amounts of Li^+ can cause harmful and detrimental effects on health, producing severe poisoning at concentrations ≥1.5 mM [2]. On the other hand, the threshold for lithium in drinking water is $8.64 \oplus 10^{-6}$ M; therefore, it is necessary to monitor its presence and detect it promptly in aqueous solutions [3]. To this end, voltammetry proved to be a useful, inexpensive and easy-to-use technique, and thus, the fine-tuning of electrochemical Li^+ detection, using screen-printed carbon electrodes (SPCEs) modified with lithium manganese oxide $LiMn_2O_4$ (LMO), is presented here [2]. Therefore, within the broader context of sustainable growth and circular economy, this study highlights first the importance of recycling spent HNT-based catalysts [1] to remove Li^+ from aqueous solutions, and, secondly, the electroanalytical approach for Li^+ detection based on linear sweep voltammetry (LSV) using LMO-SPCEs. The sensitivity of the voltammetric method was studied by placing LMO-SPCEs in solutions with various Li^{+2} concentrations ($0.2 \le mM \le 215$). A linear peak current behavior was found between $0.2 \le mM \le 21.5$, with R = 0.996. The selectivity of LMO-SPCEs toward the ion of interest (Li^+) in the presence of potentially interfering cations, such as Na^+, K^+, Ca^{2+} and Mg^{2+}, was also analyzed. With regard to the adsorption study, at pH = 7.0, the maximum adsorption capacity (q_e (mg/g)) and removal efficiency (R%) were found to be about 63 mg/g and 46%, respectively, just over 2 hours after contact between the specific adsorbent and the adsorbate. Collectively, these findings support real-world deployment of the approach, with material recycling delivering clear economic and environmental benefits.

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OR66

Breath analysis of participants of forest bathing by PTR-ToF-MS and TD-GC-MS

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Breathomics offers a non-invasive window into physiological responses to environmental exposures and health-promoting interventions. Forest bathing may benefit cardiovascular regulation and mental health [1][2]. In this study, exhaled breath from 25 participants before and after a two and a half hour forest bathing session at Parco del Respiro forest (located in the Fai della Paganella municipality, Italy at 958 m altitude) was collected into inert bags for direct analysis by PTR-ToF-MS (PTR-ToF-MS 8000, Ionicon Analytik, Austria) and compressed into sorbent tubes for TD-GC-MS (CENTRI 360, Markes International, Bridgend, United Kingdom - Agilent Technologies 8860, Santa Clara, United States). PTR-ToF-MS enabled rapid and sensitive profiling of volatile organic compounds (VOCs), while TD-GC-MS provided robust structural characterization and quantitative accuracy. PTR-ToF-MS revealed pronounced alterations in 48 m/z features following the intervention, capturing rapid and sensitive shifts in exhaled VOCs. Complementarily, TD-GC-MS offered structural resolution and quantitative accuracy, with multivariate analysis clearly separating pre- and post-Forest Bathing breath profiles. Notably, more than 20 compounds showed strong correlations across both platforms, underscoring their robustness and consistency. A comparative assessment revealed both convergences and divergences between the two platforms, highlighting their complementary strengths: real-time dynamic monitoring versus detailed chemical identification. These results demonstrated that combining PTR-ToF-MS and TD-GC-MS enhances the analytical depth of breath studies and provides an effective framework for evaluating the physiological impact of Forest Bathing.

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OR67

Surface chemistry insights into the mineral carbonation of granite scraps and Red muds, a XPS study

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As highlighted in the most recent IPCC report, the greenhouse effect is strongly linked to the continuous increase in CO_2 emissions, primarily driven by the extensive use of fossil fuels, which is contributing to global warming with severe environmental consequences [1]. Among the various research efforts aimed at mitigation, carbon mineralization, which is encompassed by CCUS (Carbon Capture, Utilization, and Storage) policies [1,2], represents one of the most promising strategies for both reducing and valorising CO_2 [1,2]. Recent studies have shown that CO_2-driven weathering processes via mechanochemical activation, involving gas–solid reactions, can lead to the formation of carbonate phases accompanied by the generation of green hydrogen and light hydrocarbons [3]. Building on this evidence, the present work investigates the reactivity of granite scraps and red muds subjected to mechanical processing, with a focus on structural transformations and gas evolution under different experimental conditions (e.g., pH, milling parameters). Experiments were performed in a modified stainless-steel jar designed to enable continuous-flow gas reactions. Structural changes and gas compositions were analysed by X-ray diffraction and gas chromatography, respectively. Preliminary results indicate that hydrogen and methane generation can be enhanced by tuning the pH of the solutions involved. Furthermore, XPS surface analysis provided insights that allowed us to propose a mechanism for mineral carbonate growth. The potential of this route for CO_2 transformation, along with related challenges, is also briefly discussed.

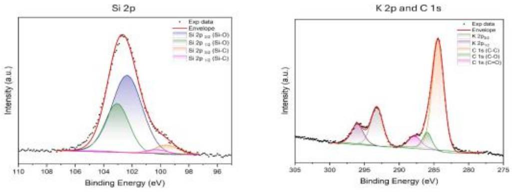

Figure 1: Experimental XPS spectra and corresponding computational fit

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OR68

NIR dyes and polyurethane matrices for colourless luminescent solar concentrators

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In 2024, photovoltaic (PV) energy accounted for 8.3% of global electricity generation[1]. Traditional PV panels may face efficiency limitations due to their sensitivity to incidence angle and shadowing, hindering their applications in the building-integrated photovoltaics field. In this context, luminescent solar concentrators (LSCs) have emerged as a promising technology. Those receive sunlight over a broad collecting surface area, converting high-energy photons into lower-energy ones *via* embedded luminophores, and guiding them by total internal reflection (TIR) towards photovoltaic cells positioned at the edges of the device[2].

Traditionally, LSC waveguides have been fabricated using glass thanks to excellent optical transparency and thermal stability. However, glass is associated to several drawbacks, including high fragility, substantial weight and limited processability[2]. In this regard, polymer-based LSCs have gained significant attention, with polymethyl methacrylate (PMMA)-based ones being the mostly spread. However, PMMA is an entirely fossil-based non-biodegradable matrix and may suffer from long-term photodegradation, limiting the sustainability and durability of the LSCs[2]. In addition, conventional LSCs commonly incorporate luminophores that emit in the visible range of the electromagnetic spectrum, resulting in overall limited device efficiencies and non-colourless panels[3].

In this work, we present different polyurethane (PU) formulations combining tunable mechanical properties, high environmental stability and bio-derived raw materials, as well as novel series of near-infrared (NIR)-emitting small molecules (SMs). In detail, we studied the effect of different polyols (*i.e.*, chemical nature and hydroxyl value) on the stabilization of the NIR-emitters in the final PUs matrix.

Acknowledgements: This research acknowledges support from the Project CH4.0 under the MUR program “Dipartimenti di Eccellenza 2023–2027” (CUP D13C22003520001). SF, GV, DC, CB acknowledge Decreto Ministeriale n. 1061 from MUR for funding the PhD scholarship.

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OR69

From molecule to device: bright Eu^{3+} supramolecular cages for aesthetically compliant photovoltaic windows

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The luminescence properties of β-diketone lanthanide complexes make them attractive to design multifunctional advanced materials, with applications spanning diversified fields, such as lasers, devices for energy harvesting, probes and sensors.

In the presented work, a family of supramolecular Eu^{3+} bis-β-diketones has been used as dopant for PMMA to produce Luminescent Solar Concentrators (LSCs). In building-integrated photovoltaics (BIPVs), LSCs are deployed as energy-producing windows capable of generating an electrical output while retaining high transparency.

The synthesized luminophores have been used to realize a series of PMMA/Eu^{3+} LSCs by cast polymerization, having a 50 × 50 mm^2 active area and thickness of 3 mm. The prepared materials strictly absorb UV photons, showing excellent aesthetic quality (AVT = 92%, CRI > 98, **Fig. 1a**), while completely blocking them, as they fully absorb AM1.5G radiation between 300 and 400 nm.

LSC-PV devices have been obtained by coupling the LSCs to Si solar cells. Electrical characterizations (J-V curves, EQE spectra, **Fig. 1b**) demonstrate that, by employing the proposed super-bright complexes, it is possible to achieve classic Eu^{3+}-based concentrators performances with a hundred-fold reduction of Eu^{3+} content. Owing to their selectivity to UV photons, the developed LSCs were investigated also as self-powered photodetectors for UV radiation, with promising preliminary results.

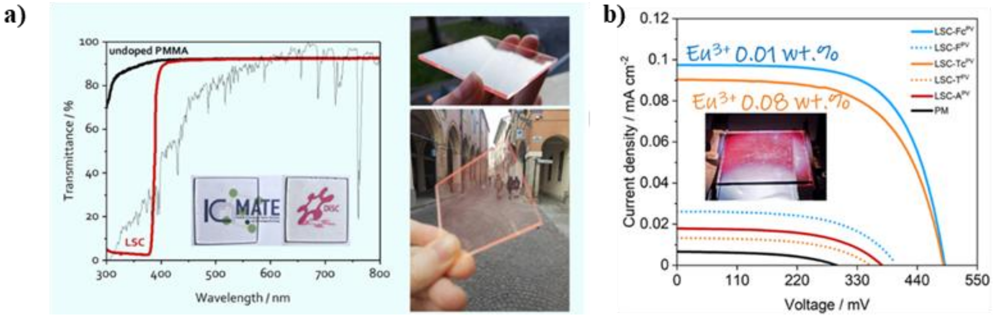

Figure 1: **a)** Transmittance spectra of the LSCs, with photographs in daylight conditions. **b)** Electrical output of the LSC-PVs under 1 sun AM1.5G illumination.

OR70

Design of deep eutectic solvent for efficient I_2 and CO_2 capture

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As industrial and economic activities continue to expand, the emissions of polluting gases remain a significant threat to the environment and human health. In the energy sector, for instance, nuclear plants produce radioactive iodine isotopes (^{129}I and ^{131}I) during uranium-235 fission, with volatile and harmful I_2 vapours requiring effective containment. Similarly, fossil fuel-based industries emit large quantities of CO_2, a major greenhouse gas responsible for global warming and climate change. Developing sustainable, reversible, and cost-effective strategies for I_2 and CO_2 capture is therefore essential. In this context, deep eutectic solvents (DESs) have attracted considerable attention in recent years due to their simpler synthesis, environmental benignity, and cost-effectiveness [1].

In this contribution, we present various cholinium-glycerol DESs with exceptional iodine uptake efficiency of up to 400 ms%, outperforming several benchmark porous absorbents. By combining Raman spectroscopy and thermal gravimetric analysis (TGA), we identified the species formed and transformed during the uptake and release of iodine, underlining the role of halogen bonding [2]. Beyond iodine, we further explored amine-based DES and DES-like systems to enhance CO_2 capture while minimizing the solvent loss commonly observed in pure amines. Absorption experiments demonstrated higher specific capacities, while TGA highlighted a remarkable reduction in evaporation, especially in the n-butylamine/glycerol mixture, likely stabilized by an extended hydrogen-bond network [3].

Together, these findings highlight DESs as a sustainable and multifunctional tool for addressing diverse industrial gas pollutants, bridging challenges from nuclear safety to carbon mitigation.

Acknowledgements: this project has received support from Project CH4.0 under the MUR program “Dipartimento di Eccellenza 2023–2027” (CUP D13C22003520001).

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OR71

Plasmonic nanomaterials for photocatalysis: morphology, dielectric environment and operando insights

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The interaction of plasmonic nanostructures with light depends strongly on morphology, size, and dielectric environment, which can be tuned to enhance reactivity [1]. Monocrystalline gold nanostructures of different morphologies (spheres, cubes, and rods) were synthesized and tested in solution-phase ferricyanide reduction to study their reactivity and stability in different localized dielectric environment. We find CTAB-capped nanocubes to be the most reactive while PVP-capped nanospheres the most stable. Complementary DRIFT spectroscopy on Pt–TiN antenna-reactor systems [2] provided molecular-level insights into CO adsorption and elementary steps under dark and illumination conditions. Further work will focus on photoelectrocatalytic glycerol oxidation using gold-based electrodes, where different nanostructure morphologies will be deposited on carbon paper to directly compare electrooxidation and photo-electrooxidation, and to elucidate mechanistic differences under illumination.

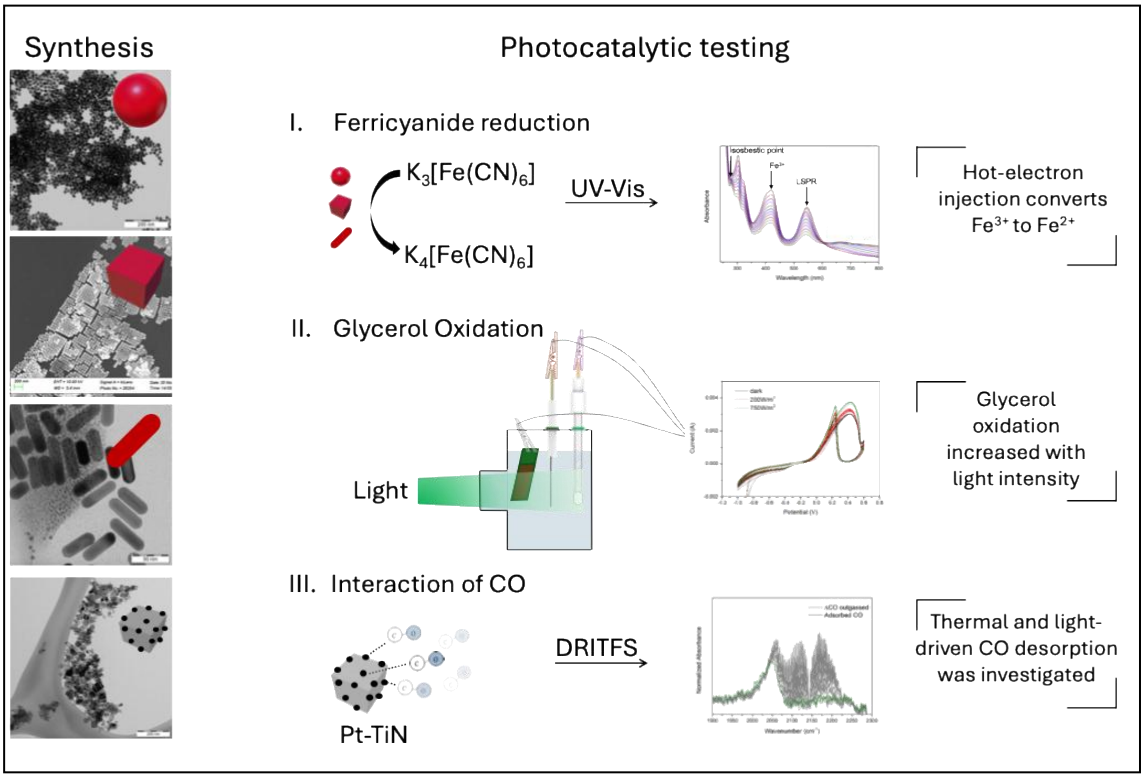

Figure 1: TEM and SEM images of the synthesized nanostructures, with a schematic summary of the photocatalytic tests

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OR72

Molecular photoswitches based on 3-benzylideneindolin-2-one scaffold as potential Combretastatin analogues

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Molecular photoswitches have emerged as an interesting research topic over the last decade due to their usefulness in several applications, such as photopharmacology [1]. In this context, the light-induced configurational changes of molecular photoswitches can modulate biological activity, enabling the development of photomediated therapies with spatial and temporal control capable of reducing the drug side effects [1].

Combretastatin A-4, a natural *cis*-stilbene derivative, presents strong inhibitory properties against tubulin polymerization, resulting on cancer cell death. However, its therapeutic application is limited by the tendency of the *cis* double bond to isomerize to the thermodynamically stable but less active *trans* form [2]. Following our recent contributions in this area [3], we have designed a novel family of molecular photoswitches inspired on Combretastatin A-4 framework, featuring a 3-benzylideneindolin-2-one core. The use of light on these compounds can induce the C=C double bond isomerization, modulating their conformation and potentially triggering an on-off cytotoxic effect.

Herein, we report the synthesis, the structural characterization and cytotoxicity evaluation of this new series. Biological assays on cancer cell lines revealed cytotoxic activity in nanomolar range for both *cis* and *trans* isomers; notably, the *trans* forms, obtained through light-induced isomerization, exhibited significantly greater potency compared to the *cis* species. Moreover, we investigated the effect of substituents on their UV–vis absorption spectra and photoswitching behavior by analyzing the diastereoisomeric compositions at the photostationary states through UV–vis and ^{1}H NMR spectroscopies. These results support the potential of this class of photoswitches as promising candidates for light-controlled anticancer therapies.

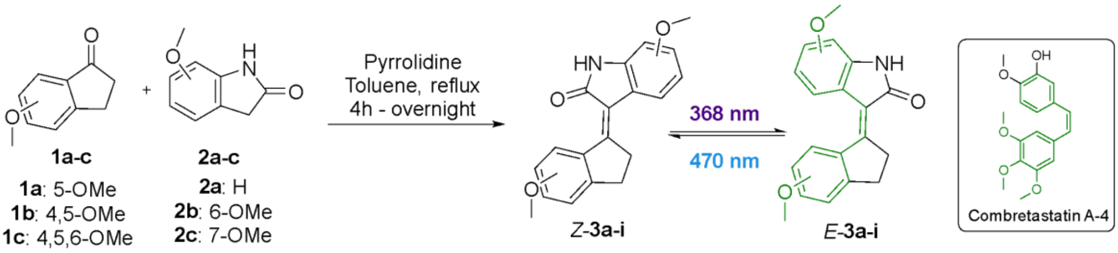

Figure 1: Synthesis of new molecular photoswitches as Combretastatin A-4 analogues.

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OR73

Development of diamino-terphenyl Covalent Triazine Polymers as visible-light heterogeneous photocatalysts

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Porous organic polymers (POPs) are a class of multi-dimensional porous materials, which are built via strong covalent linkages between various organic building blocks with different geometries and topologies [1]. Covalent triazine polymers (CTPs) belong to the family of POPs and have attracted scientific interest due to its nitrogen-rich, stable triazine rings, and favorable optical and electronic properties [2]. CTPs are insoluble in most commonly used solvent and conjugation with aromatic systems significantly enhances their chemical stability. This extended π-delocalization also imparts distinctive optical properties, making CTPs highly promising candidates for efficient photocatalytic applications.. We herein describe the synthesis of diamino-*p*-terphenyl-based Covalent Triazine Polymers in amorphous (**DAPT-CTP$_a$**) and crystalline (**DAPT-CTP$_c$**) forms through the direct nucleophilic substitution polymerization between 2,4,6-trichloro-1,3,5-triazine and 4,4″-diamino-*p*-terphenyl. Following comprehensive morphological and photochemical characterization of the two novel materials, their photocatalytic performance was assessed. DAPT-CTPs proved to be promising heterogeneous photocatalysts for visible-light-driven organic transformations, including selective oxidation of sulfides in water/ethanol and cross dehydrogenative coupling between N-aryl glycines and indoles for the synthesis of non-proteinogenic α-amino acids, affording the desire products in good or excellent yields under mild conditions.

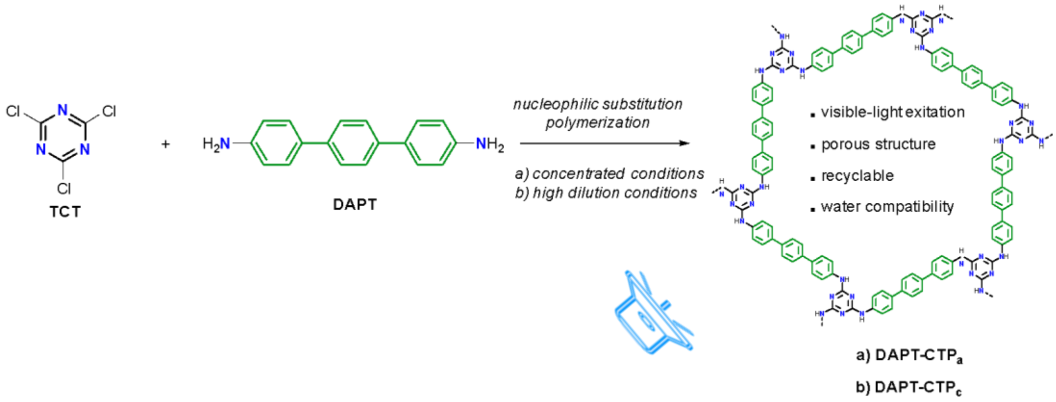

Figure 1: Development of diamino-*p*-terphenyl Covalent Triazine Polymers as heterogeneous photocatalysts

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OR74

NIR Dyes and Organic Redox Mediators for Transparent Dye Sensitized Solar Cells

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The development of integrated PV in windows/facades on buildings takes us deeper in different aspects like aesthetics, stability and performance. With Dye Sensitized Solar Cells (DSSC) is possible to offer a sustainable option for transparent and colorless windows, due to their versatility in the selection of dyes and of the electrolytes [1]. Our group synthesized some Near Infra-Red polymethine dyes [2], the best of which (VG20-C16) led us to a fully transparent and colorless DSSC reaching 80 % transmittance in complete devices using a novel hybrid organic electrolyte [3]. From this achievement, new NIR dyes were synthesized and tested in assembled devices demonstrating promising preliminary results. The other key aspect of this project is the investigation of new transparent and organic based redox mediators that have to match the energetic levels of the NIR dyes in order to regenerate them. Novel disulphide/thiol organic redox mediator were synthesized and tested, both electrochemically and photochemically demonstrating compatibility with the photosensitizers.

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OR75

On the speciation in the liquid-phase synthesis of sulfide-based electrolytes for all-solid-state batteries

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Sulfide-based thiophosphates are emerging solid electrolytes for next-generation solid-state batteries. Their physicochemical properties are highly sensitive to the chosen synthesis route, with wet-chemical methods attracting increasing attention despite limited mechanistic insights [1-2].

Herein, we report the results of our studies on the reactivity in solution of P_4S_{10} with Li_2S [3], Na_2S, K_2S, CaS, and Li_2S–Na_2S mixtures, mainly based on advanced NMR techniques. Independently of the cation, it was found that P_4S_{10} undergoes electrostatic dissolution in the presence of the sulfide salts (M_xS), leading to the formation of a novel intermediate, $P_4S_{11}^{2-}$, whose structure was confirmed by both NMR spectroscopy and single-crystal X-ray diffraction. This intermediate transforms into a range of thiophosphate species, including $(PS_3^-)_n$ polymers, $P_2S_6^{2-}$, and $P_2S_8^{2-}$, ultimately yielding the target electrolyte material.

Complementary solid-state studies confirmed that the key transformations occur predominantly in solution. These findings advance our understanding of thiophosphate chemistry and pave the way for scalable, lithium-independent synthetic approaches to solid electrolytes.

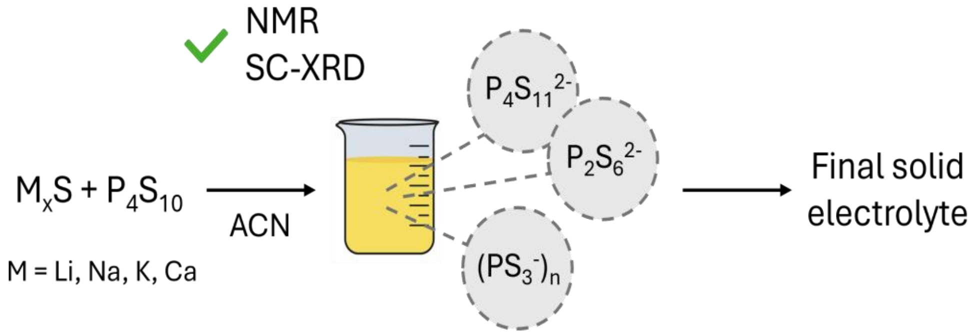

Figure 1: Sketch of the reaction between different metal sulfides and P_4S_{10}.

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OR76

Asymmetric synthesis of trifluoromethylated tetrasubstituted epoxides catalyzed by Takemoto's thiourea

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Chiral epoxides represent one of the most useful intermediates in organic synthesis, being transformed into bioactive and pharmaceutically relevant molecules [1]. The enantioselective epoxidation of alkenes can be considered the cornerstone for the asymmetric synthesis of this important class of molecules, and several methodologies were elaborated over the years [2]. However, the formation of a quaternary stereogenic center on epoxides, especially one with a trifluoromethyl motif, proves to be complicated nowadays and only a few enantioselective examples are reported in literature [3].

In this contribution, we report the first enantioselective epoxidation of trifluoromethylated tetrasubstituted acyclic alkenes (Figure 1). The corresponding products, enantioenriched epoxides bearing a quaternary stereocenter, are synthesized in excellent yield and good to high enantiomeric excess. In particular, the methodology developed exploits the use of the commercially available Takemoto's amino thiourea as organocatalyst and *tert*-butyl hydroperoxide (TBHP) as oxidant. The alkenes employed in the study were prepared by Knoevenagel condensation reaction of malononitrile with readily available aromatic trifluoromethyl ketones. Different functionalizations on the products allow the (diastereoselective) synthesis of new CF_3-containing derivatives. In addition, Density Functional Theory (DFT) studies are used to describe the reaction pathway, revealing the pivotal role of dispersion forces and halogen bonding in the stereocontrol of the reaction.

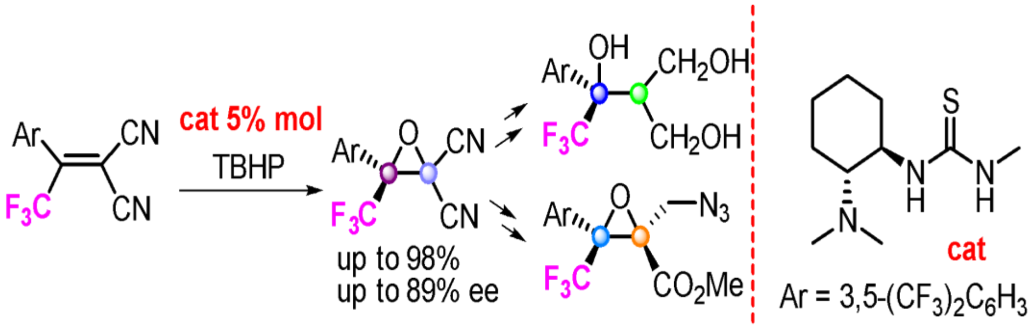

Figure 1: Takemoto's catalyst-promoted asymmetric epoxidation of trifluoromethylated tetrasubstituted acyclic alkenes and derivatization of the products.

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OR77

Effect of cerium precursor, calcination and dehydrating agents on the performance of nanostructured CeO_2 catalysts for direct synthesis of dimethyl carbonate

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Global warming and climate change, driven by rising anthropogenic CO_2 emissions, are urgent environmental challenges. Carbon Capture and Utilization (CCU) technologies offer a promising solution to reduce CO_2 concentrations in the atmosphere, with the direct synthesis of dimethyl carbonate (DMC) from CO_2 and methanol attracting significant attention within this field. DMC is a versatile chemical used as electrolyte solvent in Li-ion batteries, a building block for polycarbonates or a fuel additive. However, its direct synthesis is restricted by the thermodynamic stability of CO_2 and by the exothermic nature of the reaction, resulting in poor conversion and low yield. To overcome these issues, catalysts such as CeO_2, known for its chemical stability and good redox properties, can be employed. [1] To further enhance catalytic activity, dehydrating agents can be used to remove the water formed during synthesis and shift the equilibrium toward DMC production. In this work, CeO_2 catalysts were prepared through hydrothermal method using two different cerium precursors, ammonium nitrate and cerium nitrate. To assess the impact of calcination on the microstructural and textural properties, as well as on the catalytic performance, part of each sample was calcined and compared with the uncalcined material. The catalysts were characterized using powder XRD, Raman spectroscopy, conventional TEM, HRTEM, N_2-physisorption and CO_2/NH_3-TPD. The direct synthesis of DMC was carried out in a batch reactor, both with and without a dehydrating agent (2-cyanopyridine or methyl trichloroacetate) and products were analyzed by GC-MS. Depending on the precursor, CeO_2 with different morphologies were obtained: spherical nanoparticles for cerium ammonium nitrate and nanorods for cerium nitrate. Calcination increased the surface area, exposing more active (111) crystallographic planes and thereby enhancing catalytic performance. All the catalysts exhibited catalytic activity for the direct synthesis of DMC (2-4 $mmol_{DMC}/g_{cat}$) with yields rising to 50-70 $mmol_{DMC}/g_{cat}$ and 150-170 $mmol_{DMC}/g_{cat}$ when using 2-cyanopyridine and methyl trichloroacetate, respectively, with the calcined nanorods being the most reactive among the samples studied.

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OR78

C-H bond activation using enzyme-inspired MOF ligands for copper coordination

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The oxidation of hydrocarbons, particularly the selective functionalization of C–H bonds, remains a major goal in catalysis, with significant implications for the synthesis of high-value chemicals from simple precursors like cyclohexene. Metal-organic frameworks (MOFs) have emerged as a powerful system for the development of heterogeneous catalysts, thanks to their tuneable architectures and composition. The versatility of MOFs stems from the possibility to independently modify both metal nodes and organic linkers, allowing the fine-tuning of chemical reactivity and structural properties, providing an effective strategy to tailor catalytic performance [1].

Among the MOF families explored for catalytic applications, UiO-67 materials stand out due to their high surface area and excellent chemical and thermal stability, making them excellent candidates for designing novel catalytic systems.

This project focuses on the development of UiO-67-based catalysts specifically engineered for hydrocarbon oxidation through C–H bond activation. Taking inspiration from biological systems, our design mimics the active site of particulate methane monooxygenase (pMMO), where copper ions coordinated by histidine residues—forming the so-called "histidine brace"—play a central role in methane oxidation [2].

To replicate this coordination environment within the MOF matrix, we propose the incorporation of amino acid-functionalized linkers capable of selectively binding copper ions. This bioinspired approach aims to develop copper coordination sites that combine the catalytic advantages of enzymatic systems with the stability and recyclability characteristic of MOFs.

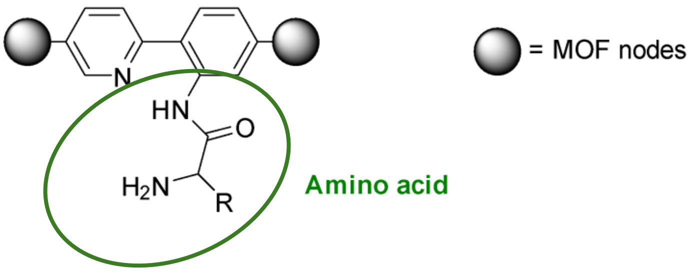

Figure 1: Amino acid-functionalized MOF linkers.

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OR79

Selective recovery of copper from waste printed circuit boards to drive methanol dehydration to dimethyl ether

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In recent years, the short lifecycle of electronic devices combined with the unrelenting advancement in modern technology has made the generation of electronic waste (e-waste) a major environmental problem [1]. One of the most diffused components of electronic equipment are printed circuits boards (PCBs) which usually contain precious metals like Cu, Ni, Fe, Au. Copper is widely used in catalysis, for example, as tuner of aluminosilicates catalytic properties. These materials, especially zeolites, are commonly employed as acid catalysts for methanol-to-olefins (MTO) reaction thanks to their strong acid sites, and the reaction course could be also driven to methanol-to-dimethyl ether (MTD) by decreasing the strength of the acid sites. In this work, copper was tested as tuner of the acidity properties of a common commercial zeolite (ZSM-5) employed in MTO/MTD reactions. Especially, MTD reaction is helpful for the ecological transition since from a sustainable feedstock as methanol (obtainable from biomass or syngas [2]) is possible to produce dimethyl ether (DME) which is a great alternative to petrol diesel, owing high cetane number and none particle matter (PM) emissions. Therefore, the first step of this work was aimed at exploring the impact of copper on the catalytic performance of zeolite ZSM-5, employing copper acetate as copper source. The second step was focused on the use of PCBs as copper source. Indeed, PCBs from old and disposed computers were collected, cut into small pieces and lixiviated. Copper was selectively extracted form the lixiviate solution using the ligand LIX-84I, and the zeolite ZSM-5 was impregnated with the obtained copper complex. The obtained final material was able to catalyze the selective conversion of methanol to DME, meanwhile by using ZSM-5 alone as the catalyst the MTO route was the preferential pathway observed.

Acknowledgements: This work has been supported under the National Recovery and Resilience Plan (NRRP), Mission 4 Component 2 Investment 1.4 – Call for tender No. 3138 of December 16, 2021 of the Italian Ministry of University and Research, funded by the European Union – NextGenerationEU [Award Number: CNMS named MOST, Concession Decree No. 1033 of June 17, 2022, adopted by the Italian Ministry of University and Research, CUP: D93C22000410001, Spoke 14 "Hydrogen and New Fuels"].

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OR80

From e-waste to catalyst: selective production of furfuryl alcohol from recovered LCO battery materials

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The rapid growth of electronic devices has led to a significant increase in end-of-life lithium-ion batteries (LIBs), resulting in large volumes of e-waste and progressive depletion of critical metals. Spent batteries remain a valuable secondary source of elements such as cobalt, nickel and manganese. Conventional recycling processes are mostly based on hydrometallurgical or pyrometallurgical routes, which require high energy input and environmental impact. In the present work, lithium cobalt oxide (LCO) based batteries were investigated, and a sustainable direct recycling strategy was developed, avoiding extreme operating conditions [1]. At the same time, lignocellulosic and agro-industrial waste has emerged as renewable feedstock for the production of bio-based compounds. In particular, hydrothermal carbonization (HTC) has been proposed as a promising route for the valorization of orange peel waste, yielding bio-oils enriched in furan derivatives [2]. Building on these two abundant sources, we propose a simple and direct methodology to convert spent LIBs into a cobalt-based heterogeneous catalyst, which was then applied to the upgrading of furan derivatives into value-added chemicals, demonstrating the potential of this sustainable recycling strategy.

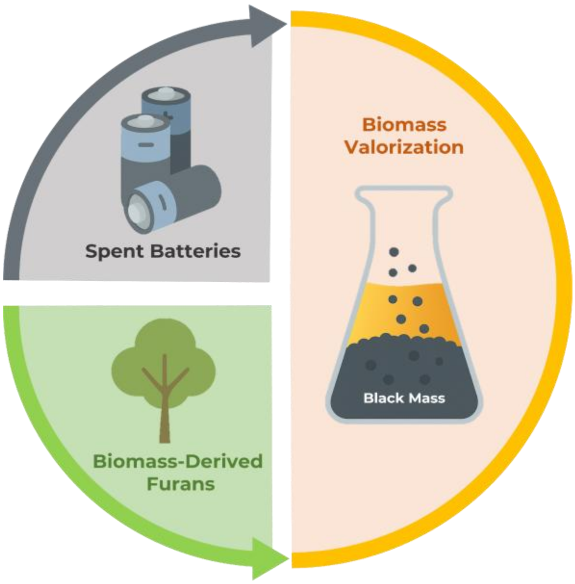

Figure 1: Overview of the general strategy: material recovery and furan upgrading

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OR81

Catalytic chemical upcycling of branched polyolefins

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The exponential rise in plastic production and consumption over recent decades has created a critical environmental challenge. Synthetic polymers are valued for their low cost, versatility, and performance, but their widespread use in short-lived applications, combined with their resistance to degradation, has led to an unprecedented waste crisis [1].

Among commodity polyolefins (POs), such as polyethylene (PE), polypropylene (PP), and polystyrene (PS), polyethylene accounts for most of the global plastic production and waste. However, its depolymerization is inherently difficult due to high thermodynamic stability and chemical inertness.

Chemical upcycling has emerged as a promising alternative to transform plastic waste into value-added products, for the synthesis of new molecules and functional materials [2]. Among the proposed routes, the polymer-to-polymer approach offers a particularly attractive solution, converting plastic waste into economically valuable polymers while retaining key physical and mechanical properties of the original material. In this contribution, we present the development of a versatile catalytic strategy for the upcycling of linear low-density polyethylene (LLDPE), offering a sustainable route toward advanced polymeric materials from plastic waste [3].

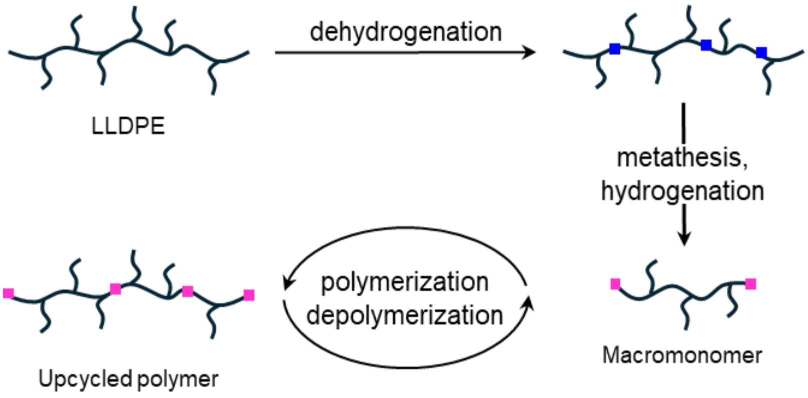

Figure 1: Proposed strategy for chemical upcycling of LLDPE plastic.

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OR82

Catalytic upcycling of polyethylene comparing different mechanochemical systems

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Global plastics production exceeded 400 million tons in 2023, of which approximately 54 million tons came from Europe (≈12.3%). Despite efforts toward greater sustainability, the share of truly circular materials remains limited: mechanical recycling contributes only 13.2% and chemical recycling just 0.2%.[1] Among polymers, polyethylene (PE) represents the most critical case: traditional mechanical processes generate lower-quality materials, while chemocatalytic strategies still rely largely on energy-intensive thermal cracking or the use of high-pressure hydrogen. In this context, hydrogen transfer catalysis with donor solvents such as 2-propanol presents a safer and more cost-effective alternative;[2] at the same time, mechanochemical activation has gained attention as a complementary, energy-efficient route capable of promoting the selective cleavage of polymer bonds under mild conditions.[3] In this study, we present the first direct comparison of different mechanochemical systems for the reductive upcycling of polyethylene (Mn ≈1700, Mw ≈4000) using a Ru/Al_2O_3 catalyst with 2-propanol as an in situ hydrogen source. A mixer mill, a planetary mill, a vibrating disc mill, and a resonant acoustic mixer were examined, evaluating their efficiency in terms of polymer conversion and liquid product distribution. Among the technologies considered, the impact mill proved to be the most efficient, achieving 30% conversion in 6 hours with a 96% selectivity towards liquid hydrocarbons in the C_5-C_{20} range, without external temperature and pressure. These data demonstrate the strong synergy between mechanochemical approaches and hydrogen transfer catalysis, outlining new opportunities for selective and energetically sustainable upcycling strategies.

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OR83

Using Artificial Intelligence to Design Novel WWP1 Inhibitors for Treating Triple-Negative Breast Cancer

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Breast cancer (BC) is the most common cancer in women and the second leading cause of cancer-related death worldwide. Among its subtypes, triple-negative breast cancer (TNBC) has the worst prognosis due to a lack of targetable markers [1]. Preclinical studies on TNBC indicated a common occurrence of diminished tumor-suppressor activity of PTEN, activating the PI3K/AKT/mTOR signaling pathway [2]. In this framework, it has been recently discovered that the ability of the proto-oncogenic E3 ubiquitin ligase WWP1 enzyme to modulate the PTEN degradation by ubiquitination [3]. Consequently, the WWP1 inhibition is considered a promising strategy to limit the cell proliferation signal consequent to the PI3K activation.

We recently applied our expertise in the computational design of bioactive peptide to generate novel peptides targeting WWP1, using AI-based algorithms combined with molecular dynamics (MD) simulations. The hexapeptide ENFA1-A demonstrated strong binding to WWP1, as confirmed by Microscale Thermophoresis (K_d = 722 nM) and Surface Plasmon Resonance (K_d = 920 nM) assays. These data were further validated by TR-FRET assays, where ENFA1-A effectively inhibited WWP1 enzymatic activity, displaying an EC_{50} of approximately 5 μM. Notably, MTS assays showed that ENFA1-A exhibited a stronger dose-dependent response than the reference compound indole-3-carbinol (I3C) in MCF7 and MDA-MB-231 of BC and TNBC cells, respectively. The identification of novel WWP1 inhibitors aimed at fighting TNBC has the potential to transform the treatment paradigm for this aggressive subtype of cancer, offering promising prospects for the development of new anticancer protocols characterized by lower toxicity and improved patient outcomes, such as improved life expectancy.

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OR84

PISA-Engineered Polymeric Nanoparticles for the Targeted Delivery of FS536, a Doxorubicin–Nitric Oxide Hybrid with Anti-MDR Activity

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Our research group has developed a promising molecular hybrid, FS536, by conjugating doxorubicin (DOXO), a widely used chemotherapeutic agent, with a nitric oxide (NO) donor prodrug [1]. This hybrid is capable of simultaneously releasing both DOXO and NO through the activation of specific enzymatic pathways. Biologically, FS536 combines the classical cytotoxic activity of DOXO with the redox-modulating effects of NO. In vitro studies have further demonstrated that FS536 can overcome one of the major mechanisms of multidrug resistance (MDR) associated with DOXO treatment. This effect is attributed to the ability of NO to nitrate efflux pumps involved in MDR, specifically MRP1, thereby inhibiting their function. To further enhance FS536's bioavailability, improve its targeting capacity, and maximize therapeutic efficacy while minimizing systemic side effects, polymeric nanoparticles were designed, synthesized, and characterized using the PISA (Polymerization-Induced Self-Assembly) method. These nanoparticles are capable of encapsulating FS536 within their core. Preliminary results support the potential of these nanosystems as innovative platforms for more selective and effective anticancer therapies based on FS536.

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OR85

Novel SARS-CoV-2-$\mathrm{PL}^{\mathrm{pro}}$ chemical cluster: from identification to optimization

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The natural evolution and drug-induced mutations of SARS-CoV-2, a *β* coronavirus responsible for COVID-19, have resulted in the continuous outbreaks of new variants, highlighting the urgent need for the development of broad-spectrum antiviral agents [1]. Within this context, our research, as part of the EU-funded AVITHRAPID project [2], focuses on the development of new antiviral compounds targeting the SARS-CoV-2 papain-like protease ($\mathrm{PL}^{\mathrm{pro}}$), a key enzyme in viral replication and in host immune evasion by cleaving post-translational modifications, such as ubiquitin and ISG15 [3]. Starting from $\mathrm{PL}^{\mathrm{pro}}$ hits identified through high-throughput screening conducted by the European Lead Factory, several novel chemical clusters with nanomolar/micromolar potency and high selectivity were selected. Our current efforts are focused on structure-activity relationship (SAR) studies on one of these clusters (Figure 1). In this work, we will present the screening results, the synthetic strategy and the biological evaluation. These results represent a key step toward the identification of a novel class of inhibitors against SARS-CoV-2, with the potential to also target other coronaviruses.

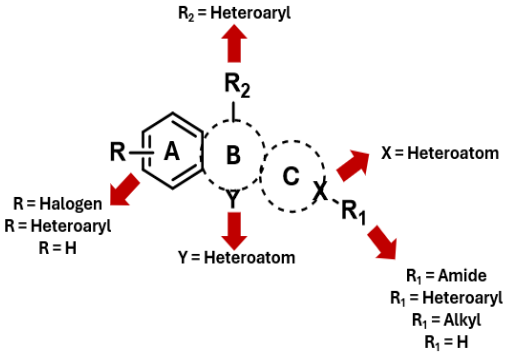

Figure 1: General SAR studies on cluster under investigation

The project, being part of AVITHRAPID, is funded by the European Union under grant agreement No 101137192.

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OR86

Leveraging nature as source of potential anti-Alzheimer's drugs: The NInFA project

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Alzheimer's disease (AD) is a multifactorial condition that is currently considered a global emergency due to its significant economic and social impact [1,2]. Currently, the few available drugs could only improve the symptoms with a minor influence on the progression of the disease [1]. In recent years monoclonal antibodies, such as Lecanemab, have been developed as the first disease-modifying agents, even if their use is not yet common due to the high costs and serious side effects [1]. Following a different approach, the ambitious goal of discovering new potential small molecules with anti-AD activity is the point of the PRIN PNRR 2022 NinFA project (Nature-Inspired structures: Fungal metabolites for a sustainable semi-synthetic approach to the discovery of new multi-target anti-Alzheimer's drugs) [3]. Specifically, we planned to leverage nature as a source of chemical scaffolds for the semi-synthesis of new molecules with anti-AD potential multi-target activity.

The project activities allowed the development of an innovative process for the extraction and purification of ochratoxin A from extracts produced by selected high producing microfungi strains using environmentally friendly methodologies such as the use of Deep Eutectic Solvents (DESs) and hydroalcoholic mixtures.

The obtained OTA were employed as the starting point to obtain Ot-alpha, the key natural scaffold to be included the final hybrids, through the combination with different fragments from classical anti-AD drugs (e.g. donepezil and rivastigmine) [1,2].

All the synthetic pathways involved have been optimized applying green chemistry principles by using neat reactions, hydroalcoholic mixtures and DESs, reducing the use of volatile solvents when possible [3]. The potential biological activity of the different hybrids will be evaluated through in vitro assays against classic and innovative targets [1-3].

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OR87

Purine-based compounds as potential REXO2 inhibitors

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Since cancer is one of the most leading causes of death, it represents a global health issue. Consequently, the search for new anticancer drugs is a complex challenge of great interest for medicinal chemistry.

Currently, it has become clear that mitochondrial function is essential for the viability of cancer cells. In this contest, mitochondrial ribonucleases are essential to ensure mitochondrial RNA (mtRNA) maturation. Irregular mtRNA processing and decay is linked to pathological conditions such as chronic inflammation and ageing [1]. Non-coding RNAs fragments are degraded as single monophosphate nucleotides by REXO2, an exoribonuclease mainly working in mitochondria. It has recently been demonstrated that REXO2 is overexpressed in several cancers [2]. REXO2 can catalyze the hydrolysis of 2-5 nucleotides nanoRNA (and also DNA), with the highest affinity (nM) for 2 nucleotide substrates [3]. Due to its relevance in sustaining proliferation, REXO2 represents a promising target for the discovery of novel mitochondrial targeted anticancer-drugs.

The goal of this work was to design purine-based compounds able to specifically inhibit REXO2, with the aim to interfere with cell proliferation. The synthesized compounds were evaluated *in vitro* and their effect tested on prostate cancer cell line DU145. Moreover, formulation studies have been done for the delivery of the most promising compound into the mitochondria through liposomes. Liposome systems have been formulated with phospholipids composition using different methods to obtain the best encapsulation of the purine-based compound, and dequalinium chloride has been used for the selective delivery of the drug into mitochondria. The drug-loaded liposomes were tested on DU145 and on the breast cancer cell line 231-BR. This study represents the first approach for the synthesis of potential REXO2 inhibitors.

Acknowledgments: PRIN 2022, funded by the European Union – NextGenerationEU – Project N. 2022KC3X9L CUP N. J53D23009040006

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OR88

Folding Interfering small Molecules as next-generation therapeutics for AKT1-driven diseases

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The PI3K/AKT/mTOR pathway is a key driver of cancer, and oncogenic mutations in AKT1, particularly the recurrent E17K variant, promote tumorigenesis and therapy resistance [1]. This mutation is also associated with the rare pediatric disease Proteus Syndrome [2]. To date, the only approved AKT-targeted drug is **capivasertib**, an ATP-competitive inhibitor whose efficacy is limited by isoform and mutation selectivity. To overcome these limitations, we investigated the selective degradation of AKT1-E17K using Folding Interfering small Molecules (FIMs) through PPI-FIT (Pharmacological Protein Inactivation by Folding Intermediate Targeting) technology [3], which exploits transient folding intermediates as druggable conformations. By shifting the paradigm from inhibition to degradation, the PPI-FIT approach offers a novel route for mutant-specific targeting of AKT1.

Ribosome-assisted folding simulations revealed 13 conformations of an AKT1-E17K folding intermediate, guiding AI-driven virtual screening of a 5-million-compound library. Multiparametric filtering yielded 203 candidates for experimental testing. Primary screening with a novel BiFC-based assay - Light Identification of Protein Suppressors (LIPS) - identified 9 FIMs capable of reducing intracellular AKT1-E17K levels at micromolar concentrations. These hits are currently undergoing confirmation and further mechanistic characterization.

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OR89

Rearming the toolbox against Monkeypox: new tecovirimat analogues for target exploration

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Among emerging and re-emerging viral threats, Monkeypox virus (MPXV) has gained significant attention in 2024 due to the rise of a newly identified clade in regions where it was previously nonendemic [1]. A member of the Orthopoxvirus genus within the Poxviridae family, MPXV is currently classified into two main clades (I and II), with subclades (Ia-b, IIa-b) mainly differing in their geographic distribution, clinical presentation, and virulence. Following the global eradication of smallpox, MPXV has become the most relevant orthopoxvirus affecting human health. However, the missing cross-protection from smallpox vaccination, coupled with a lack of preventative immunization in younger populations and limited therapeutic options, has intensified the search for new antiviral strategies in the concept of preparedness. Currently available antiviral agents targeting MPXV, primarily acting on viral DNA polymerase or the p37 envelope protein, face challenges related to clinical efficacy on late treatments and emerging resistance [2]. In this context, the development of new molecular tools is essential to advance our understanding of viral targets and optimize drug design. For these reasons our research group has developed a novel library of tecovirimat analogues, in an effort aimed at broadening the structure–activity relationship (SAR) landscape and facilitating target exploration in MPXV research. These analogues were evaluated through phenotypic antiviral assays, leading to the identification of a promising lead compound, spirovirimat, with notable inhibitory activity. Complementary in silico studies provided further insights into the potential mechanism of action and validated the hypothesized molecular target as the same as tecovirimat. This work not only introduces new chemical entities with improved synthetic accessibility but also provides valuable tools for probing MPXV biology. Our findings contribute to a growing body of knowledge essential for guiding the development of next-generation antivirals and improving preparedness against future orthopoxvirus outbreaks.

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Flash presentations

FL01 – Federica Borzelli (UniROMA1)

FL02 – Francesca D’Ambrosio (UniROMA1)

FL03 – Silvia Picello (UniMIB)

FL04 – Aafia Sehar (UniPV)

FL05 – Sara Camorali (PoliMI)

FL06 – Gioele Ancora (UPO)

FL07 – Marco Marinsalta (PoliMI)

FL08 – Leonardo Sparascio (UniBO)

FL09 – Arianna De Santis (PoliMI)

FL10 – Gloria Nicastro (PoliMI)

FL11 – Maria Gentile (UniPD)

FL12 – Nicole Canzian (UniVE)

FL13 – Lorenzo Filidei (UniPI)

FL14 – Gioele Foltran (UniVE)

FL15 – Sara Sajied (UniCAM)

FL16 – Sanam Gull Arshad (UniSA)

FL17 – Tommaso Castiglia (UniBA)

FL18 – Riccardo Ciciriello (UniBA)

FL19 – Michela Galli (UniMI)

FL20 – Gabriele Maria Gargano (UniPA)

FL21 – Marta Ippolito (UniPA)

FL22 – Chiara Lenzi (UniBO)

FL23 – Elison Lepore (UniCAM)

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FL25 – Annunziata Francesca (UniMI)

FL26 – Paolo Reale (UniPA)

FL27 – Sara Venturi (PoliTO)

FL28 – Sara Vllahu (UniSA)

FL29 – Filippo Lugli (UniMORE)

FL30 – Alessandra Glovi (UniNA)

FL31 – Chiara Grassi (UniMORE)

FL32 – Carla Aliberti (UniNA)

FL33 – Hiba Ali (PoliTO)

FL34 – Daniel Augusto Machado Alencar (UniTO)

FL35 – Gabriele Manenti (UniSI)

FL36 – Francesco Riina (UniFE)

FL37 – Arianna Giacchero (UniTO)

FL38 – Francesco Ricco (UniTO)

FL39 – Sharon Silloni (UniPG)

FL40 – Marianna Barbieri (UniPD)

FL41 – Carmen Corea (PoliMI)

FL42 – Vincenzo Roselli (UniBA)

FL43 – Elettra Della Ceca (UniCAM)

FL44 – Andrea Gotti (UniMI)

FL45 - Mehdi Moayedi (UniPD)

FL46 - Chiara Billi (UniNA)

FL47 - Alessia Bono (UniPA)

FL48 - Sara Cascone (UniBO)

FL49 - Veronika Kost (UniTS)

FL50 - Gabriele La Monica (UniPA)

FL51 - Francesca Mancuso (UniME)

FL52 - Beatrice Di Mattia (UniROMA1)

FL53 - Alessia Lanzini (UniMI)

FL54 - Leonardo Milioni (UniSI)

FL55 - Clara Mocchetti (UniMI)

FL56 - Mirko Pineschi (UniSI)

FL57 - Giorgia Tempra (UniMI)

FL01

Unveiling Aptamer Features and Selectivity through Molecular Dynamics: The Case of OBA3

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Aptamers are short single-stranded nucleic acids synthesized via the SELEX process. Their ability to fold into complex three-dimensional structures and bind target molecules with remarkable specificity make them promising tools for biosensing, diagnostics, and drug delivery. In this work, we performed a computational study of the Ochratoxin A Binding Aptamer 3 (OBA3), a DNA 19-mer which selectively binds the mycotoxin ochratoxin A (OTA) over its close and less toxic analogue ochratoxin B (OTB) [1]. OTA and OTB differ by only a single atom, with Cl in OTA replaced by H in OTB. This difference likely accounts for their distinct binding profiles, as halogen bonding interactions can play a decisive role in molecular recognition.

We combined classical molecular dynamics (MD) simulations and alchemical free-energy calculations to investigate the structural and thermodynamic basis of OBA3 selectivity. Halogen bonding was carefully modeled by mimicking the chlorine *σ-hole* with an extra point of charge (dummy atom) [2].

Our analysis showed that the binding of either OTA or OTB markedly reduces the conformational flexibility of OBA3, constraining the aptamer into more compact states compared to its free form, consistent with the ligand-induced folding observed in many aptamers. Alchemical free energy calculations correctly predicted OBA3's stronger affinity for OTA and provided an estimation of the relative free energy of binding.

Altogether, our results highlight the potential of MD in unveiling both the structural and thermodynamic determinants of aptamer specificity, thereby offering valuable guidance for the rational design and optimization of aptamers.

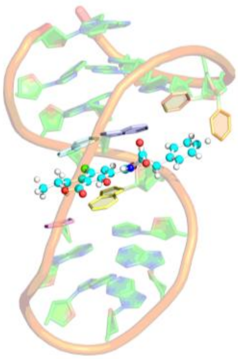

Figure 1: Snapshot of the OBA3-OTA complex from MD simulations.

[1] G. Xu, J. Zhao, N. Liu, M. Yang, Q. Zhao, C. Li, and M. Liu, *Nucleic Acids Res. 47* (2019) 5963–5972.
[2] M. A. A. Ibrahim, *J. Comput. Chem.* 32 (2011) 2564–2574.

FL02

A computational approach to the study of carbon nanodots for the determination of their structure and properties

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Since their discovery in 2004, carbon nanodots (CNDs) have emerged as a promising class of carbon-based nanoparticles due to their properties: intense photoluminescence, low toxicity, excellent biocompatibility and easy surface functionalization [1]. Their synthesis employs straightforward bottom-up and top-down methods, which dictate the functional groups present on their surface, their size and their photoluminescent response [1]. As a result, CNDs have found numerous applications, particularly in biological and biomedical fields [1]. Despite extensive experimental and computational studies, a comprehensive atomic-level understanding of their structural features and their correlation with optical properties remains incomplete [2]. To fill this gap, an explicit treatment of the electronic degree of freedom is required, along with a compatible computational method that balances efficiency and accuracy.

Here, we present results on the application of a computational multiscale approach based on *ab-initio* DFT (Density Functional Theory) and semi-empirical (TB-DFT, tight-binding density functional theory) methods to the class of CNDs. The challenge lies in identifying more effective starting models than the ones currently used, which are mostly based on polycyclic aromatic hydrocarbons (PAHs) [3]. We propose that progressively larger carbon clusters (CCs) can serve as effective structural models for CNDs, as shown in the figure reported below.

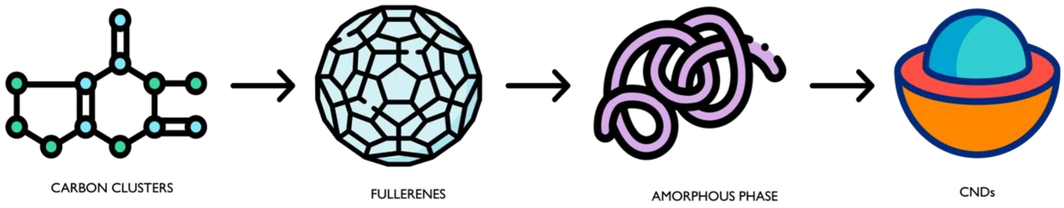

Figure 1: Graphical representation of the structural evolution of structural models for carbon nanodots.

[1] D. Ozyurt, M. AlKobaisi, and R. K. Hocking, *Carbon Trends* 12 (2023) 100276.
[2] K. J. Mintz, M. Bartoli, and M. Rovere, *Carbon* 173 (2021) 433–447.
[3] M. Langer, M. Paloncýová, and M. Medveď, *Applied Materials Today* 22 (2021) 100924.

FL03

Single-atom catalysts on goldene

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In single-atom catalysis, the interaction between isolated metal atoms and the supporting matrix plays a pivotal role in determining the stability and reactivity of the system. This has driven the search for novel supporting materials, particularly 2D materials, where graphene stands out. Simultaneously, increasing attention is being given to Single-Atom Alloys (SAAs), a subclass of Single-Atom Catalysts (SACs) where the supporting matrix is a metal itself. Recently, Kashiwaya et al [1] reported the synthesis of goldene, a self-standing 2D monolayer of Au(111), the gold analogue of graphene. Motivated by this breakthrough, we explored a new class of SACs consisting of transition metal (TM) atoms stabilized on goldene. The atomistic nature of Au-ene requires simulations, where we rely on VASP with a PBE+U functional. We identified several systems that remain stable under both reducing and oxidizing conditions [2]. We then investigated their catalytic performance in the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER), discovering that certain TM-goldene systems exhibit promising activity, with reactivity significantly different from the same TMs supported on bulk Au(111). Our analysis included a comprehensive evaluation of potential reaction intermediates, extending beyond the conventional species typically assumed in HER and OER [3]. This study provides strong theoretical evidence that SACs embedded in goldene could offer promising stability and catalytic reactivity.

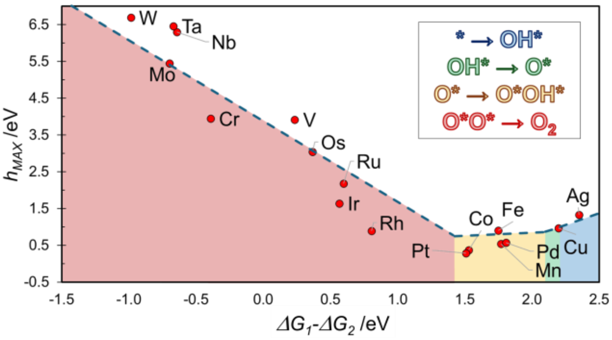

Figure 1: Calculated h_{MAX} for all the OER species presented in this work. Different colored areas correspond to the formation of different intermediates as indicated in the inset.

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[2] G. Di Liberto, L. Giordano, G. Pacchioni, *ACS Catal.* **14** (2024) 45.
[3] I. Barlocco, L.A. Cipriano, G. Di Liberto, G. Pacchioni, *J. Catal.* **417** (2023) 351.

FL04

Reaction mechanisms and kinetics of the OH-initiated atmospheric degradation of acrolein and its geminal diol

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Volatile organic compounds (VOCs) are important atmospheric species that serve as precursors of secondary organic aerosols, which influence both air quality and climate. Within this group, carbonyl compounds, such as aldehydes, are especially important due to their enhanced reactivity. Once in the atmosphere, they can react with hydroxyl radicals following either H-abstraction or OH-addition pathways, or they can undergo hydration in cloud droplets or aerosols leading to their corresponding geminal diol forms. In the current work, we focus on the OH-initiated degradation of both acrolein ($CH_2=CH–CHO$, 2-propenal) and its geminal diol ($CH_2=CH–CH(OH)_2$, 2-propene-1,1-diol) [1].

In order to clarify the mechanisms involved in the atmospheric gas-phase reactions, a detailed quantum-chemical investigation including all possible H-abstraction and OH addition routes is first performed. Specifically, the potential energy surfaces (PESs) are constructed by optimizing geometries and computing zero-point vibrational energies at the DSDPBEP86-D3/jun-cc-pVTZ level of theory, while electronic energies are refined using the “jun-cheap” composite scheme (jChS) [2]. As a second step, rate constants for the dominant pathways are computed employing canonical variational transition state theory (CVTST) for paths with distinct barriers, and eventually variable-reaction-coordinate transition state theory (VRC-VTST) for those involving submerged transition states [3]. It is shown that the dominant channels involved H-abstraction from the aldehydic site and OH-addition to the α- and β-carbon atoms. Moreover, abstraction of the H-atom adjacent to the carbonyl group in acrolein gives a less stable radical than same abstraction from the geminal diol. As a third step, the subsequent oxidation of the formed geminal diol radicals by molecular oxygen (O_2) is investigated eventually resulting in the formation of acrylic acid.

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[2] V. Barone, J. Lupi, Z. Salta, N. Tasinato, *J. Chem. Theory Comput.* 17 (2021) 4913-4928; S. Alessandrini, V. Barone, C. Puzzarini, *J. Chem. Theory Comput.* 16 (2020) 988-1006.

[3] J. L. Bao, D. G. Truhlar, *Chem. Soc. Rev.* 46 (2017) 7548-7596.

FL05

Doubling down on Bispidines: Novel Tetratopic Ligands for Coordinative Polymerization

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Refineries, as well as the chemical, pharmaceutical, and automobile industries, along with various human activities, release significant amounts of volatile organic compounds (VOCs) such as halogenated hydrocarbons, aldehydes, and aromatic compounds, which pose environmental and human health risks[1]. With VOC emissions projected to reach 60 teragrams of carbon per year by 2030, effective sequestration strategies are urgently needed. Coordination polymers (CPs) represent a class of hybrid metal–organic materials self-assembled from two components: metal ions and organic ligands[2]. While three-dimensional coordination polymers 3D CPs, particularly metal-organic frameworks (MOFs) have long held a prominent role in VOC adsorption applications, recent efforts have shed light on CPs that lack inherent porosity or possess small, tunable pores and cavities with size and shape complementarity to specific guest molecules. Moreover, although MOFs have traditionally been constructed using simple ligands, the incorporation of structurally complex compounds has emerged as a promising strategy to broaden the scope of accessible materials. Among these, bispidine-based ligands, derivatives of 3,7-diazabicyclo[3.3.1]nonane, have been employed in the synthesis of one-dimensional CPs that exhibit effective and selective VOC adsorption under ambient conditions. The rigid yet versatile bispidine scaffold, capable of supporting significant structural modifications, represents a highly attractive platform for the design and development of novel coordination polymers[3].

In this work, we have designed and synthesized tetratopic bispidine ligands which have been then used to obtain novel CPs (Figure 1). They have been synthesized, characterized by SC- and P-XRD and tested for VOCs adsorption applications.

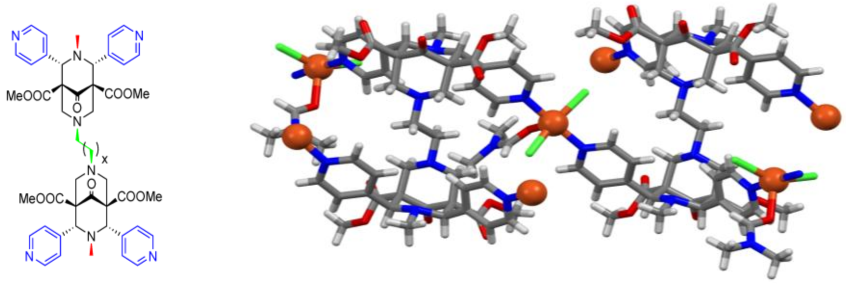

Figure 1: a) Tetratopic bispidine ligands (x = 1-4) and b) Representative 1D coordination polymer obtained with Cu(II) and L1 (x =1).

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[2] Lippi, M.; Cametti, M. *Coordination Chemistry Reviews* **2021**, 430, 213661.
[3] Sayed, A.; Cametti, M., *Chemistry A European J* **2024**, 30 (40), e202401464.

FL06

Top-down strategies for tailoring porosity in zeolites: comprehensive evaluation of structural and adsorption properties.

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Hierarchical zeolites, characterized by the presence of interconnected micropores and mesopores, are versatile materials capable of overcoming the typical limitations of microporous systems, including poor mass transfer, hindered diffusion, and strict product selectivity [1,2]. One possible route to obtain hierarchical porous materials is through top-down approaches, in which secondary porosity is introduced through post-synthetic modification of a pre-existing microporous matrix. In this study, commercial HZSM5 and HUSY zeolites (SiO_2/Al_2O_3 = 80, MFI and FAU frameworks, respectively) and a natural clinoptilolite (HCLI, Si/Al = 5, HEU framework) were desilicated using NaOH solutions at different concentrations. The resulting hierarchical structures were characterized by XRD, N_2 physisorption at 77 K, TGA and FTIR spectroscopy of adsorbed probe molecules to assess the nature, strength and accessibility of the acid sites (Figure 1A,A’). Their performance in Cu^{2+} and Co^{2+} ions removal from aqueous solution was then evaluated by UV–Vis spectroscopy. Selectivity tests were also carried out to determine the materials' affinity for the target ions. The three zeolites exhibited distinct adsorption behaviors: HZSM5 demonstrated the highest adsorption capacity but showed no specific affinity for either metal ion, in contrast to HUSY and HCLI, which displayed a clear preference for Co^{2+} (Figure 1B). Notably, the desilication treatment significantly enhanced the adsorption efficiency of the studied materials. Dr. Gioele Ancora acknowledges financial support from the Next Generation EU – MUR PhD career grant.

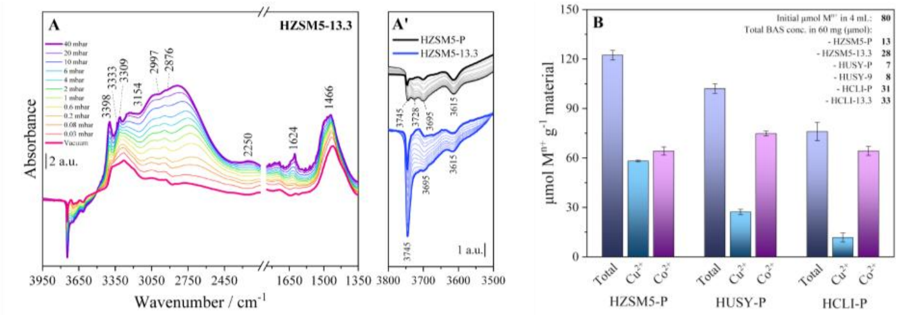

Figure 1: FTIR difference spectra of NH_3 adsorbed on hierarchical HZSM5 at room temperature (A); comparison of HZSM5 spectra before and after desilication in the OH stretching region (A’); Amount of M^{n+} captured by the studied zeolites from aqueous solution after 24 hours, expressed as µmol g^{-1}(B).

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[2] S. Mitchell et al. Nat. Commun. 6 (2015) 8633-8647.

FL07

Modelling of electrochemically enhanced leather tanning

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This work focuses on the optimization of the leather tanning phase, the crucial part of the process that transforms the raw material into the finished product, bringing in the leather substances that can attach themselves to the collagen fibres and make the material durable. Today, the most used tanning agent is basic chrome sulphate due to its affinity with the carboxyl groups of the collagen chains. Just before tanning the skin is immersed in an acid solution, this facilitates the entry of chromium into the hide. This phase is known as pickling. The pH value is then restored to the starting one to ensure proper fixation of the tanning agent. This step before tanning is necessary because it makes the adsorption of chromium onto the collagen fibres thermodynamically disadvantaged. Consequently, the tanning agent can move freely in the leather. To optimise the process, the entry of chromium into the leather must be improved. This is done by exploiting the electrical charge of the chromium ions and facilitating its entry by applying an electric field. In this work, modelling of the phenomenon was conducted. The adsorption of chromium on the skin is a phenomenon that has received little attention in the literature, so it was necessary to conduct an experimental campaign to find the parameters of the adsorption isotherm. This made the modelling results closer to the real ones. The model develops the Nernst Planck equation and considers the change in diffusivity as the chromium concentration changes. Given the high responsivity of acid in the case of electric field application, the possibility of combining pickling, tanning and basification in a single step is explored. The system consists of two partial differential equations (PDE). Their resolution allows the behaviour of chromium over time and its local distribution within the leather to be known. The results are very satisfactory and show the high rate of entry of the tanning agent and the precision with which the concentration profile in the skin can be controlled. Comparing the numerical value of the members that make up the equation governing the phenomenon reveals the total prevalence of the input due to the applied electric field. In conclusion, the results obtained are compared with experimental data from research conducted in parallel to this study within the same research group and a great agreement between them is noted.

FL08

Life Cycle Assessment of An Environmentally Sustainable Approach for Metal Recovery from Battery Cathode Production Scraps

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As the global demand for lithium-ion batteries accelerates, driven by the growth of electric vehicles and renewable energy systems, the sustainability of battery metal sourcing is critical. Recycling end-of-life batteries offers a promising strategy to reduce reliance on primary raw material extraction and alleviate associated environmental and geopolitical concerns. However, conventional recycling processes often rely on harsh chemicals, toxic solvents, and energy-intensive steps that undermine their environmental benefits. In this study, a novel and environmentally conscious recycling process for lithium cobalt oxide (LCO) cathode materials was developed using green solvents, including triethyl phosphate (TEP) and deep eutectic solvents (DES). To evaluate the environmental performance of the proposed process, a comprehensive Life Cycle Assessment (LCA) was conducted. This assessment was used to identify the main environmental hotspots within the process units. Following this, a contribution analysis was performed to determine which flows (e.g. materials, energy, waste) contribute most significantly to the overall environmental impact.

Acknowledgements We acknowledge for financial support the projects: "RELY: Transformation of REcovered/recycled spent Lithium-ion Battery cathodes into porous materials for high power-energy storage" (MAECI-Italy South Africa Grande Rilevanza bilateral project); "DiGreen: a digital and chemical approach for green recycling of Li-based batteries" funded by the European Union - Next Generation EU, Missione 4 Componente 1 Project CUP J53D23008790006, and MOST—Sustainable Mobility Center project, funded by the European Union Next-Generation EU (PIANO NAZIONALE DI RIPRESA E RESILIENZA (PNRR) e MISSIONE 4 COMPONENTE 2, INVESTIMENTO 1.4 e D.D. 1033 17/06/2022, CN00000023.

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FL09

Exploring the potential of nanocellulose as coating agent for enhanced barrier performance of paper-based materials

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The intrinsic porosity of paper-based materials poses significant challenges for their use in packaging applications, as it results in poor barrier properties against water, oil, and gases. Consequently, high coating loadings are often required to achieve the desired performance. Simultaneously, the worsening environmental concerns associated with conventional petroleum-based packaging materials are driving research toward the development of more sustainable alternatives. In this context, cellulose, the most abundant biopolymer on Earth, is gaining increasing attention due to its low cost, biodegradability, and renewability [1,2]. In addition, its hierarchical structure enables the extraction of nanoscale constituents with high surface area and strong hydrogen bonding capability, making them promising candidates for enhancing barrier properties of paper-based materials [3]. In this study, various nanocellulose-based coating agents are developed and applied to different paper substrates to improve barrier properties against water, oil, and gases (figure 1). Nanocellulose materials are obtained through different extraction methods and subsequently formulated into low-consistency coating agents.

Remarkable results are achieved even at low coating loadings (<5 g/m^2), including complete air resistance (below 0.08 μm·Pa^{-1}·s^{-1}) and grease barrier performances (kit 12). Furthermore, functionalization with various lipophilic moieties is carried out to modulate the inherently hydrophilic nature of nanocellulose, thereby improving water resistance. Water contact angle measurements and Cobb60 test are performed to assess the hydrophobic behaviour of paper coated with functionalized nanocellulose, reaching outstanding results.

Finally, different application techniques are tested to study how the coating deposition method influences barrier performance.

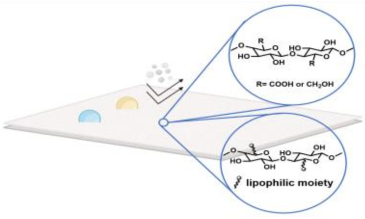

Figure 1: Graphical abstract

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FL10

Cellulose-based nanosponges loaded with hydrophobic eutectics: breakthrough solutions for water remediation

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Clean water is a fundamental goal of the 2030 Agenda for Sustainable Development and the European Green Deal's Zero Pollution Action Plan, making water remediation a critical focus in research. Conventional extraction techniques like dispersive liquid-liquid and solid-liquid microextraction (DLLME and DSLME) face challenges, including the use of volatile organic solvents and non-sustainable sorbents with limited capacity.

This study addresses these challenges by introducing new classes of sustainable materials based on hydrophobic non-ionic eutectic solvents (HES) [1]. HES offer several advantages, including being chloride-free, easy to prepare from natural precursors, 100% atom economy, and high sustainability [2]. Preliminary studies with HES composed of terpenes, long chain carboxylic acids and phosphine oxides have demonstrated promising extraction abilities in water remediation from phthalates and bisphenol A.

To expand their use, HES-loaded cellulose nanosponges (HECS) are produced. HECS are hybrid materials composed of HES in combination with cellulose nanosponges (CNS). CNS are eco-safe nanostructured materials made from TEMPO-oxidized nanocellulose and different crosslinkers [3], a particularly attractive option for sustainable water remediation.

The materials' structure and extraction mechanisms are thoroughly investigated using SEM and compression analyses together with NMR and UV-Vis spectroscopy. This comprehensive analysis, combined with a high material tunability, allows for precise control over their properties, making these materials highly adaptable for various water remediation applications.

The development of HES-based hydrophobic CNS marks a breakthrough in sustainable water treatment. By overcoming the limitations of current extraction methods, this research offers a safer, more efficient, and eco-friendly solution for removing harmful contaminants. These materials have the potential to play a crucial role in achieving global clean water goals and advancing the field of green chemistry.

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[2] D. O. Abranches, and J. A. P. Coutinho, *Curr Opin Green Sustain Chem.* 35 (2022) 100612.

[3] A. Fiorati, G. Grassi, A. Graziano, G. Liberatori, N. Pastori, L. Melone, L. Bonciani, L. Pontorno, C. Punta, and I. Corsi, *J. Clean Prod*. 246 (2020) 119009.

FL11

Development of bio-based PLA thermosets with chemical recycling potential

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The transition toward a circular economy presents a major challenge for the polymer sector, particularly for thermosets, which lack sustainable end-of-life options due to their crosslinked structures, which hinder recycling [1]. Furthermore, most commercially used thermosets are derived from fossil-based feedstocks, often toxic raising serious environmental and health concerns and underscoring the urgent need for safer, sustainable alternatives [2]. Covalent adaptable networks (CANs), crosslinked via dynamic covalent bonds, offer a promising solution, combining adaptability with chemical recyclability [3].

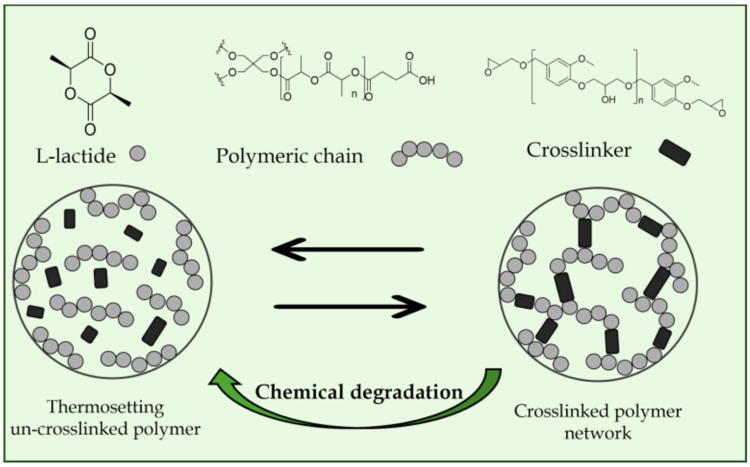

Figure 1: A new synthetic strategy for thermosets polymer with a circular life cycle

In this contribution, we investigate poly(lactic acid) (PLA) as a sustainable platform for synthesizing thermosets using non-toxic, bio-based crosslinkers. We also explore strategies for chemically degrading the thermosets to enable material recovery. This approach aims to combine bio-based origin with recyclability and circularity potential.

Acknowledgement This study was carried out within the Next Generation EU, Partenariato esteso PE0000004 "MICS–Made in Italy Circolare e Sostenibile", project "ULISSE", PNRR, CUP D43C22003120001.

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FL12

Management of plastics waste and development of sustainable biocomposites: an approach for the circular economy

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The growing global production of plastics, estimated at approximately 368 million tons annually, has made the transition to a Circular Economy model indispensable, where waste is not seen as a final product to be disposed of, but as a resource to be valorized. In this context, fossil-based plastics represent a complex and hardly biodegradable waste, with high potential environmental impact if not managed correctly [1]. A sustainable transformation of the plastics sector requires a strategic vision built on two complementary pathways.

The first involves optimizing the recycling and reuse of conventional polymers. Advanced mechanical and chemical recycling technologies play a key role in converting heterogeneous and contaminated plastic waste streams into high-quality secondary raw materials, thereby reducing the dependence on virgin resources and minimizing landfill or incineration.

The second pathway focuses on the development of more sustainable alternatives. Although bioplastics currently account for only 1% of global plastic production, they offer distinct advantages in reducing dependence on fossil resources and lowering greenhouse gas emissions, aligning with the European Union's sustainability goals. Biocomposite materials emerge as a promising replacement for fossil-based materials, especially if based on biodegradable polymer matrices such as polybutylene succinate (PBS), whose thermomechanical properties are comparable to polypropylene and whose monomers can be bio-based [2]. The addition of natural fillers, derived from waste biomass, can reduce costs, polymer content and modifying the final material's properties. Notably, algae that accumulate as waste along marine coastlines represent a sustainable biomass source for use as filler. Their growth does not compete with the food supply chain and their use contributes to the reduction of eutrophication phenomena, while also helping to clean up beach environments [3].

The transition to sustainability in the plastics sector requires a strategic vision that integrates two fundamental paths: the optimized management and recycling of traditional plastic materials and, at the same time, the development and implementation of innovative, sustainable materials like biocomposites. This dual approach is key to a successful transition toward a circular economy with reduced environmental impact.

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FL13

NMR characterization of HA-BDDE hydrogels and prospective functionalization with pH indicators

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Hyaluronic acid (HA) is a naturally derived biopolymer widely employed in the biomedical field for the development of hydrogels with high biocompatibility and tunable viscoelastic properties. The degree of crosslinking, and the specific substitution site of the linker on HA functional groups, influence the mechanical performance and clinical applicability of the resulting materials [1].

In this study, HA hydrogels were prepared by crosslinking with 1,4-butanediol diglycidyl ether (BDDE) under different conditions and operative systems. The resulting HA-BDDE networks were characterized by nuclear magnetic resonance (NMR) spectroscopy. ^{1}H NMR analysis allowed the identification of diagnostic signals corresponding to BDDE-derived crosslinks and polymer backbones. Quantitative integration of specific resonances enabled the estimation of the degree of crosslinking, the degree of modification, and the position of the linker across the different formulations [2].

An additional perspective of this work concerns the incorporation of pH-responsive indicators into HA-BDDE hydrogels, with the aim of designing “smart” wound dressings capable of signaling bacterial infection through a visible color change. Possible strategies include physical entrapment or covalent binding of the indicator during hydrogel preparation. In this context, NMR is considered a key tool to clarify whether the dye interacts physically with the polymer matrix or becomes chemically integrated into the crosslinked network.

This combined approach highlights the potential of NMR for both optimizing biomaterial final properties and confirming the integration of functional molecules such as pH indicators. The resulting multifunctional systems represent promising candidates for advanced wound care, drug delivery, and regenerative medicine.

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FL14

Study of bio-based fillers and additives for the production of biodegradable biopolymers

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Beer spent grain (BSG), the primary by-product of brewing processes, represents an underutilized, cost-free, and abundantly available resource for biorefinery applications. In this study, BSG has been exploited for the first time as a bio-filler (BSGF) in polybutylene succinate (PBS)-based polymer matrices to develop novel bio-composites (PBS-BSGF). This approach enables the reduction of virgin biomass and fossil-derived polymer consumption by converting agro-industrial waste into a high-value material. Furthermore, BSG has been investigated as a renewable source for the synthesis of bio-based compatibilizers. Typically, bio-composites require the addition of compatibilizing agents (often fossil-derived) to bridge the polarity gap between the apolar polymer matrix and the polar filler [1]. The lipid fraction of BSG was chemically modified to obtain amphiphilic molecules capable of improving polymer-filler interfacial adhesion. Oleic and linoleic acids were initially employed as model compounds for the synthesis of candidate compatibilizers via esterification and epoxidation reactions [2,3]. Subsequently, lipids were extracted from BSG using organic solvents and subjected to the same functionalization procedures. All synthesized additives were characterized through NMR, FT-IR, and elemental analysis. A series of PBS/BSG composite formulations were developed with and without the incorporation of additives, and their performance was evaluated using DSC, ATR-FTIR, TGA, and SEM techniques. This study presents the first integrated valorization of an agro-industrial by-product as both a filler and a compatibilizer in the development of biodegradable polymer composites.

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FL15

Development of bio-stimulating nanofibrous scaffold via Electrospinning from Polymer/Cyanobacterial extracts solution

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Electrospinning is a versatile technique used to produce polymeric nanofibers with high surface-to-volume ratios, ideal for advanced applications such as controlled release systems and bio-functional materials [1]. This study presents an innovative approach that integrates biologically derived components from mass cultures of the cyanobacterium *Trichormus variabilis* into polymer nanofibers to create functional scaffolds for potential use as bio-stimulants in the agri-food sector. *T. variabilis* was chosen for its ease of growth, nitrogen-fixing ability, and production of extracellular polymeric substances (EPS), which enhance plant growth, stress tolerance, and soil fertility [2]. Nanofibers were fabricated by electrospinning polyethylene oxide (PEO) solutions using the cyanobacterial extract as solvent. The extract, obtained by autoclaving and centrifuging *T. variabilis* cultures, retains inorganic salts and potentially bioactive compounds from cell lysis, such as amino acids. Controlled cultivation ensured consistent extract composition. Morphological and elemental analyses (FE-SEM / EDX) confirmed the formation of uniform, defects-free fibers below 500 nm in diameter and the successful incorporation of nutrients into the fibers. This work highlights the potential of converting cyanobacterial extracts into valuable nanostructured scaffolds for controlled delivery of bio-stimulants, promoting a sustainable approach.

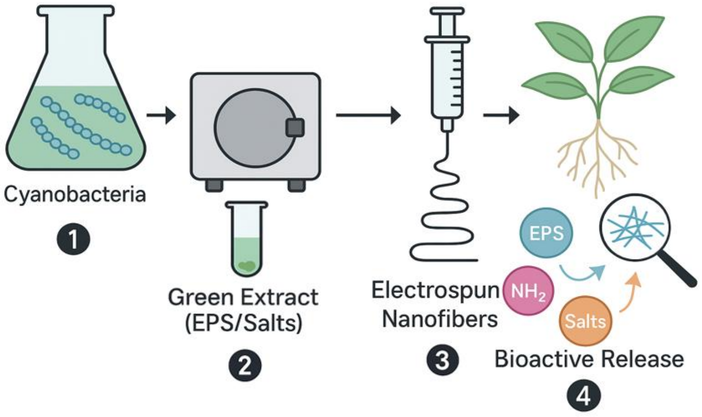

Figure 1: Scheme of nanofiber fabrication: Cyanobacterial extract is combined with PEO after cultivation and autoclaving. Fibers are obtained via electrospinning.

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FL16

Vinylogous aldol reaction of isochroman-3,4-dione

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The isochroman scaffold is an important structural motif found in a variety of bioactive natural compounds and synthesized pharmaceuticals, making it a well-known heterocyclic molecule in drug development and a key contributor to pharmacological progress [1,2]. In this study, we provided an efficient and ecologically friendly synthesis of isochroman-3,4-dione, a useful derivative of isochroman, with a good 87% yield. The reactivity of the synthesized dione was then carefully studied under mild reaction conditions to determine its potential for further derivatization and functionalization. Our research found that when the dione was deprotonated with triethylamine (Et_3N), it quickly generated a nucleophilic enolate intermediate. The enolate intermediate also went through a vinylogous aldol reaction with aromatic and aliphatic aldehydes, resulting in more structurally complicated derivatives. These reactions were efficient, with yields of up to 80% with aromatic aldehydes and up to 90% with aliphatic aldehydes. These intriguing findings demonstrate isochromanone-3,4-dione's outstanding synthetic flexibility, establishing it as a valuable and easily available intermediate for the rapid production of structurally varied and possibly bioactive compound

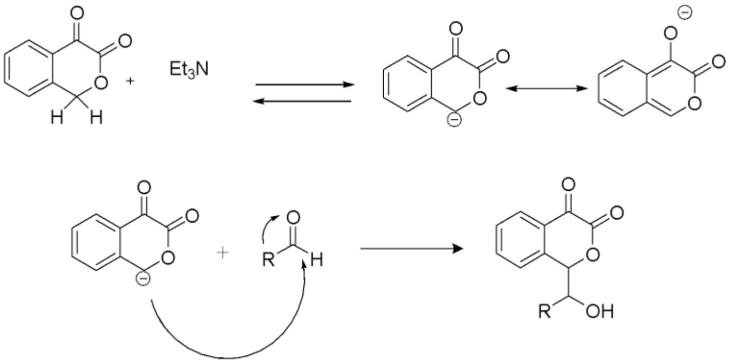

Figure 1: Scheme of vinylogous aldol reaction of isochroman-3,4 dione .

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FL17

o-Methyl choline acetate as a novel reaction media for Pd@slag catalyzed Heck cross-coupling: a renewable and efficient new pathway

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Transition-metal-catalyzed cross-coupling methodologies, including the Mizoroki–Heck reaction, are cornerstone strategies in C–C bond construction for the synthesis of fine chemicals and pharmaceutical intermediates. However, their environmental footprint, driven by the use of expensive noble metals, volatile organic solvents, and homogeneous non-recyclable catalysts, represents a critical challenge. Herein, we report a green and renewable-based approach to the Mizoroki–Heck reaction, employing biodegradable ionic liquids as reaction media and an unconventional catalyst derived from industrial residues. Steel slag, a by-product of steelmaking process generated in millions of tons per year, was repurposed as a heterogeneous support for palladium [1], producing Pd@slag via impregnation with only 2% w/w Pd. The catalytic system, composed of Pd@slag and choline-based ionic liquids, was tested in the Mizoroki–Heck coupling of aryl iodides and aryl bromides with alkenes under mild conditions [2].The reactions were carried out in synthetically accessible and biodegradable ionic liquids, including choline acetate, choline bromide, and methylated choline acetate. Substrate scope screening revealed broad applicability, with good to exceptional yields across various substrates. Recycling experiments confirmed the robustness and stability of the entire catalytic system, which maintained its performance over multiple runs with negligible palladium leaching. The Pd@slag/ionic liquid system not only replaces conventional expensive catalyst supports and hazardous solvents but also opens new pathways for the development of greener and cheaper synthetic methodologies in transition-metal catalysis.

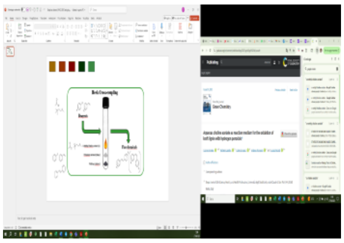

Figure 1: Pd@slag catalyst for Heck cross couping in o-MeChAcO.

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FL18

Palladium-Catalyzed Buchwald-Hartwig Amination Assisted by Infrared Irradiation

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The Buchwald-Hartwig amination, palladium complexes catalyzed, is a highly efficient and versatile methods for forming C(sp^2)–N bonds.[1] With its broad utility, from drug discovery to materials science, it enables the synthesis of advanced functional materials. In recent years, the growing demand for cleaner and more sustainable chemical processes has driven the search for alternative energy sources to conventional thermal heating. While techniques such as microwave irradiation and mechanochemical activation have received considerable attention, infrared (IR) irradiation has remained largely underexplored, despite being a clean and efficient mode of reaction activation that aligns well with the principles of green chemistry. As part of our ongoing research into IR-assisted synthetic methodologies,[2] here in, we report an innovative and environmentally friendly protocol for Pd-catalyzed Buchwald-Hartwig amination under IR irradiation.[3] This method features quasi-solvent-free conditions, tolerance to atmospheric moisture and oxygen, and employs cyclopentyl methyl ether (CPME), a biodegradable and non-peroxide-forming ether, as a minimal reaction medium. The protocol demonstrates a broad substrate scope, effectively coupling a wide range of aryl iodides and bromides bearing electron-donating or electron-withdrawing groups with both primary and secondary amines. Excellent conversions and isolated yields were achieved within significantly reduced reaction times.

These findings position our IR-assisted Buchwald–Hartwig amination protocol as a sustainable and attractive alternative to conventional thermally driven approaches, offering a promising path forward for environmentally responsible synthetic organic chemistry.

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FL19

Functionalization of E3 ligase recruiters in the green solvent Cyrene: a sustainable approach for the synthesis of PROTACs precursors

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Proteolysis Targeting Chimeras (PROTACs) are heterobifunctional molecules able to induce the degradation of a protein through the Ubiquitin Proteasome System (UPS). PROTACs are made of a ligand of the protein of interest (POI), a ligand of an E3 ligase (e.g. Cereblon, CRBN, or Von Hippel Lindau, VHL) and a flexible linker necessary to connect the two moieties [1].

Although the POI ligand is target-specific, the same E3 ligase ligand fragment—identical in chemical structure—is used across many PROTACs; therefore, greener functionalization strategies can be broadly applied. Typically, E3 ligase recruiters such as VH-032-Me and lenalidomide (Figure 1) are derivatized via amide coupling, whereas F-thalidomide is usually functionalized through nucleophilic aromatic substitution (S_NAr). Both transformations are often carried out in DMF or DMSO, solvents classified as reprotoxic (H360), and should therefore be avoided when possible. The green solvent Cyrene has gained popularity in recent years as an environmentally sustainable replacement of high temperature boiling organic solvents. Derived from cellulose, Cyrene is a non-toxic, non-mutagenic and biodegradable solvent; its high water miscibility allows for straightforward removal via aqueous workup [2].

In this work, we explored the functionalization of CRBN and VHL recruiters in the green solvent Cyrene. Different reaction conditions were explored and optimized, screening also alternative energy sources, among which ultrasounds. This allowed us to obtain a library of E3 ligase ligands derivatives, bearing the main functionalities commonly used to assemble PROTACs.

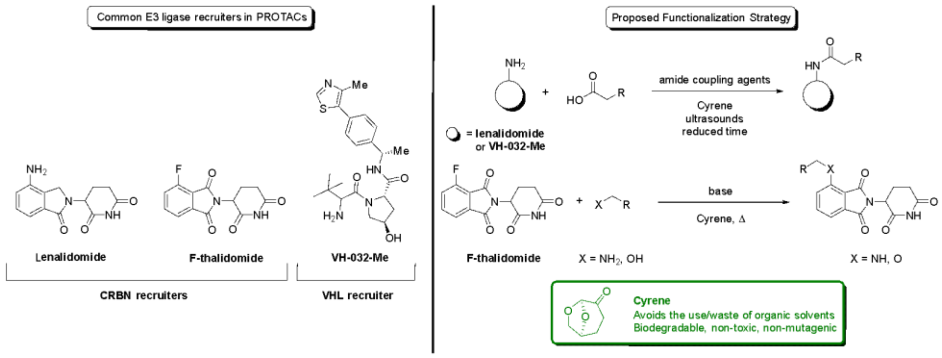

Figure 1. Left panel: common CRBN and VHL recruiters used for PROTACs synthesis. Right panel: functionalization strategies of the selected ligands in Cyrene.

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FL20

Carbon nano-onion/poly ionic liquid/POM hybrid as recyclable catalyst for the oxidation of alcohols

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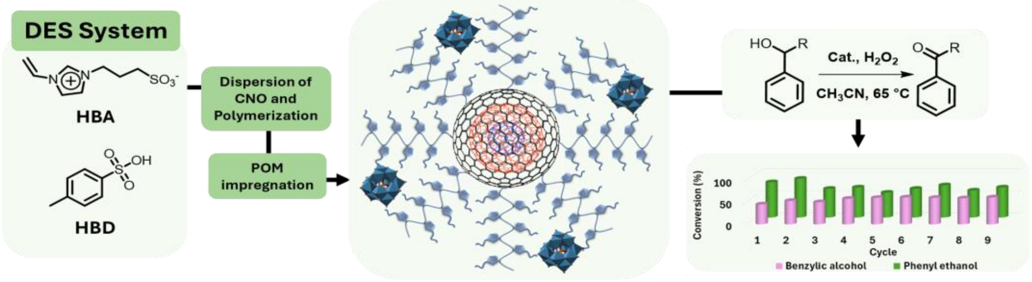
A new green and efficient way for the production of Carbon nanoform (CNF)-based hybrid catalysts is here presented [1]. The increased use of CNFs as supports in hybrid materials is due their great mechanical and thermal stability, lightness and particularly for their well-defined geometries [2]. Our group developed a simple and practical way for their functionalization with a procedure that requires the use of peculiar solvent systems: Deep eutectic solvents (DES) in which one of the components is a polymerizable ionic liquid, usually an imidazolium salt. These solvent systems can both act as a good dispersion media for the CNFs, which is one of the most common challenges to face with these kinds of supports, and they also actively take part in the functionalization reaction: the polymerizable salt is allowed to grow directly onto the carbonaceous surface, which then acts as a templating agent. Using this procedure the CNFs gain a compact coating consisting of a Poly(ionic liquid). It's a versatile process that allows to obtain not only different functional groups in the final material, such as amine, carboxyl or sulfonic groups, but also different morphologies depending on the nature of the monomer: using mono- or bis-vinyl imidazolium salts it is possible to obtain respectively linear or cross-linked polymeric coatings.

Using this procedure, we developed a catalyst composed of Carbon nano-onions coated with a linear polymer with sulfonic functionalities onto which we anchored a tungsten Polyoxometalate. With the so obtained catalyst we performed oxidation of alcohols into aldehydes or ketones. The material showed moderate conversions but mainly a great recyclability, basically maintaining its activity up to 9 cycles.



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FL21

Probing Ni in co-doped $LaFeO_3$ Perovskites by Synchrotron X-ray Absorption Spectroscopy

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Nickel is a highly catalytically active, abundant, and cost-effective metal, representing a promising alternative to noble metals such as Rh, Ru, and Pt. Nickel-doped perovskite oxides have recently gained significant attention for their potential in advanced catalytic applications, particularly in solid oxide fuel cells (SOFCs) and solid oxide electrolysis cells (SOECs). While Ni incorporation enhances oxygen vacancy formation, promotes oxygen ion transport, and improves the oxygen reduction reaction (ORR) kinetics, uncontrolled Ni doping may also induce impurity phases (e.g., NiO), ultimately degrading electrochemical performance.

In this work, we present a systematic investigation of $LaFeO_3$ perovskites co-doped with Ni and Mo at the B-site, and Ba and Ca at the A-site. Using synchrotron-based X-ray absorption spectroscopy (XAS) at the European Synchrotron (ESRF), we directly probe the local environment of Ni to unravel how the presence and type of different dopants influence its structural and electronic behavior. This study provides critical insights into the mechanisms governing Ni stabilization within the B-site of the perovskite lattice. Preliminary results indicate that Mo co-doping enhances Ni incorporation into the perovskite lattice, while suppressing NiO segregation. By identifying the optimal doping strategy, our results pave the way for the rational design of highly stable and efficient Ni-based perovskite catalysts for next-generation energy conversion technologies. [1] [2]

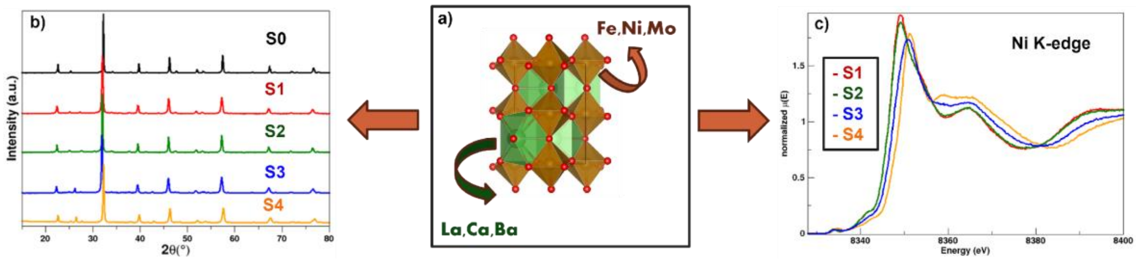

Figure 1: Samples: (**S0**) $LaFeO_3$, (**S1**) $LaFe_{0.85}Ni_{0.075}Mo_{0.075}O_3$, (**S2**) $La_{0.95}Ca_{0.05}Fe_{0.85}Ni_{0.075}Mo_{0.075}O_3$, (**S3**) $La_{0.85}Ca_{0.075}Ba_{0.075}Fe_{0.85}Ni_{0.075}Mo_{0.075}O_3$, (**S4**) $La_{0.8}Ca_{0.1}Ba_{0.1}Fe_{0.85}Ni_{0.075}Mo_{0.075}O_3$. a) Graphical representation of orthorhombic $LaFeO_3$; c) (b) XRD patterns; (c) Ni K-edge HERFD-XANES spectra.

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FL22

Efficient Ruthenium-Catalyzed Guerbet Reaction for Bioethanol Upgrading to Higher Alcohols

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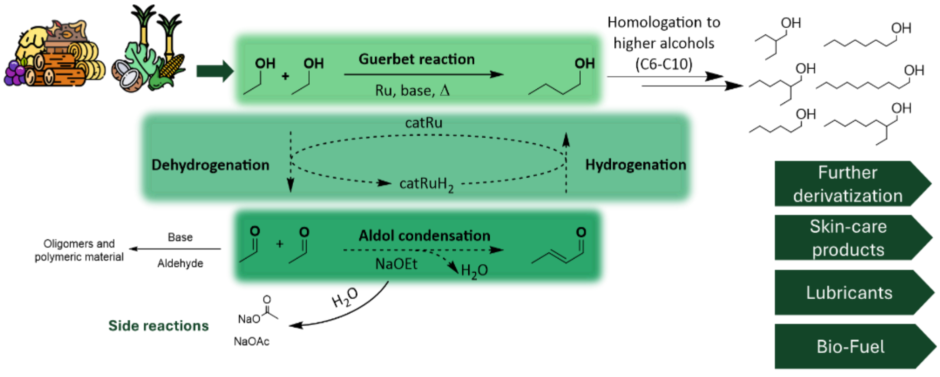
With global bioethanol output a significant renewable resource, its conversion into valuable chemicals, beyond its biofuel role, is crucial. The Guerbet reaction, which transforms ethanol into higher alcohols like butanol, represents a key pathway involving sequential dehydrogenation, aldol condensation, and hydrogenation.[1] Our work at Professor Mazzoni's lab has centered on homogeneous ruthenium catalysts for this transformation, yielding good ethanol conversion and butanol selectivity. Critically, the incorporation of a co-catalyst proved instrumental in enhancing selectivity towards longer-chain alcohols. This effective catalytic system was also validated in upscaling studies, where adjustments to reactor configuration led to improved carbon balance, indicating strong potential for the practical implementation of our catalyst. Utilizing a synergistic approach combining computational modeling and experimental validation, we successfully elucidated the catalytic mechanism, including how the co-catalyst contributes to improved selectivity. [2] Moreover, the integration of microwave irradiation as a heating source drastically reduced reaction times from hours to minutes, significantly improving the overall sustainability and throughput of the process.



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FL23

Novel Double-Brønsted acidic deep eutectic solvents and their applications as solvents and catalysts in chemical transformations

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During the last years, the number of Deep Eutectic Solvents (DESs) liquids are increasing in the literature due to the high quantity of molecules capable of H-bonding that allow to obtain stable liquids by mixing binary systems[1]. In this work, the crossing points of theoretical melting curves has been used to identify and determine a new and peculiar class of DESs: double Brønsted-acid DESs, mixtures of two Brønsted-acid molecules[2]. These DESs were identified comparing the experimental and the theoretical melting curves and by using ionic conductivity measurements. The catalytic properties of DESs are related to the properties of the forming molecules[3], therefore these novel DESs were tested as acidic reaction media in model reactions. Double Brønsted-acidic DESs gave excellent results in the Claisen-Schmidt transformation, while in the synthesis of indole from alkynes the products were obtained without using any metal or other catalyst for the first time to our knowledge.

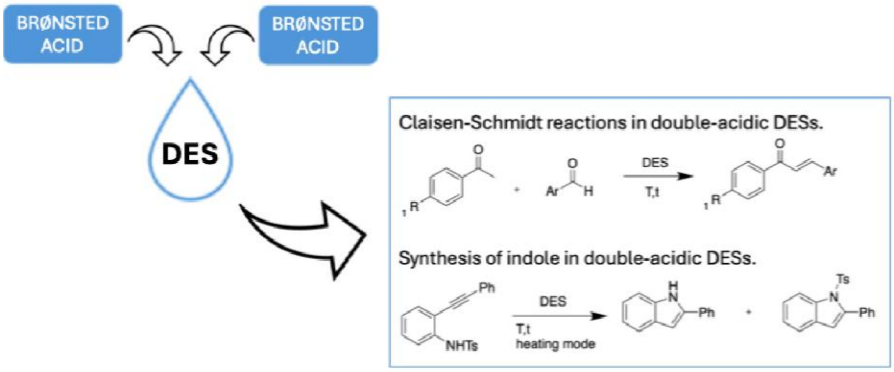

Figure 1: Claisen-Schmidt reactions and Synthesis of indole in double-acidic DESs.

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FL24

Towards sustainable API production: lidocaine synthesis in deep eutectic solvents

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The pharmaceutical industry is under increasing scrutiny to minimize its environmental impact, particularly in the synthesis of Active Pharmaceutical Ingredients (APIs), which are typically resource-intensive and generate substantial waste. Green Chemistry (GC) offers sustainable alternatives, with Deep Eutectic Solvents (DESs) emerging as a promising class of eco-friendly solvents [1,2]. DESs, composed of natural, renewable compounds, provide low toxicity, biodegradability, and tunable properties, making them an attractive alternative to conventional solvents.

In this work, we present a green approach for the synthesis of lidocaine, a widely used local anesthetic and antiarrhythmic drug, using biobased DESs. The traditional synthesis of lidocaine involves acylation of 2,6-dimethylaniline followed by amidation with diethylamine, often using toxic solvents and moisture-sensitive reagents [3]. We demonstrate that DESs can replace these traditional solvents, providing an efficient and environmentally benign reaction medium. The use of DESs enhances the solubility and stability of key intermediates, improving overall reaction efficiency and yield.

Our results show that the incorporation of DESs into lidocaine synthesis not only reduces solvent waste but also supports a more sustainable and efficient production pathway. This approach exemplifies the potential of DESs to enable greener pharmaceutical manufacturing, offering a viable alternative that aligns with global sustainability goals and regulatory trends.

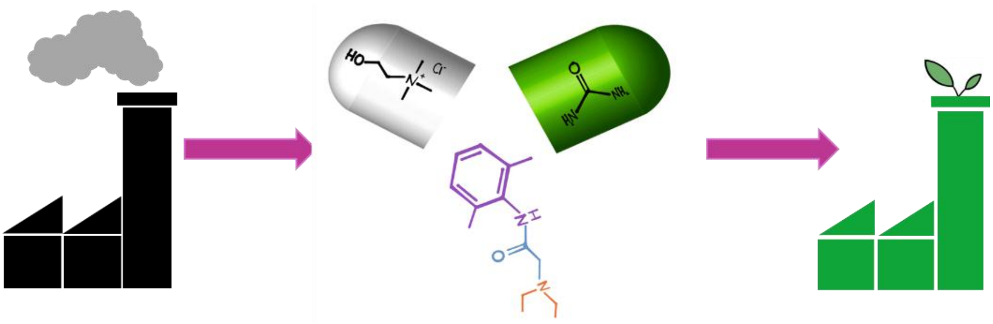

Figure 1: DES-mediated lidocaine synthesis

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FL26

Melamine-amino acid based eutectogel as reusable catalyst for aldol reaction

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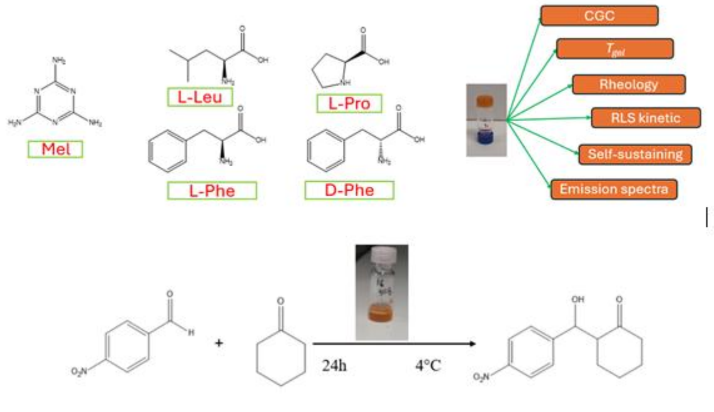
Controlling stereoselectivity during a chemical reaction is extremely important. Carbon–carbon (C–C) bond formation reactions often lead to asymmetric molecules that are essential to the synthesis of many compounds of pharmaceutical interest [1]. One of the principal strategies to control stereoselectivity in chemical reactions is the use of a chiral catalyst. Supramolecular gels can act as heterogeneous catalysts with interesting properties such as self-reparation capabilities, which are absent in conventional heterogeneous catalytic systems [2]. In this work, we explored the possibility to obtain catalytic eutectogels using composites of Melamine (Mel) and amino acids in a 2:1 molar ratio in a deep eutectic solvent, choline chloride: triethylene glycol (1:3) (ChCl:TEG). Amino acids investigated were L-proline (L-Pro), L-leucine (L-Leu), L-phenylalanine (L-Phe) and D-phenylalanine (D-Phe). For each gel, we determined gel-sol transition temperature (T_{gel}), gelation time and aggregated sizes, performing resonance light scattering (RLS) kinetics. In addition, for these gels, rheological measurements and self-sustaining tests are conducted. These eutectogels were used as heterogeneous catalysts for aldol reaction between *p*-nitro benzaldehyde and cyclohexanone.



The best catalyst was the L-Pro based gel. The best performance in terms of yield (around 70%), conversion (> 80%) and stereoselective control, syn/anti ratio (75/25) and enantiomeric excess (80%) was obtained at 4 °C for 24 hours without stirring. In addition, the catalyst was reused five times without significant decrease in terms of conversion and stereoselective control.

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FL27

Coupling TiO_2 with $CuInS_2$ Quantum Dots toward solar CO_2 reduction

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The reduction of atmospheric CO_2 has become a major scientific and technological challenge, leading to intensive research on photocatalytic materials inspired by natural photosynthesis. Artificial photosynthesis provides a sustainable route to convert CO_2 and water into fuels and value-added chemicals using solar energy [1]. Titanium dioxide (TiO_2) is one of the most studied photocatalysts due to its stability and abundance, but its efficiency is limited by fast electron-hole recombination and weak visible-light absorption. In this work, we focus on the synthesis and characterization of anatase/rutile TiO_2 through an innovative free template synthesis method to enhance its photocatalytic performance compared with commercial P25 TiO_2. The role of calcination in polymorphic formation was investigated by comparing calcined and non-calcined TiO_2: XRD analysis revealed a mixed anatase/rutile composition (A = 88,8%, R = 11.2%), calcination did not significantly change the phase composition but improved crystallinity, while HRTEM images provided particle size distribution information.

To overcome TiO_2 limitations we coupled it with $CuInS_2$ (CIS) quantum dots (QDs) (TiO_2/QDs 10:1), aiming to extend light absorption into the visible–NIR range and improve charge separation. CIS QDs with a high surface-to-volume ratio, tunable band gaps and low toxicity, makes them suitable for enhancing the photocatalytic response of TiO_2 [2]. N_2 adsorption/desorption analysis at 77K revealed a reduction in in textural properties after coupling with CIS QDs: the specific surface area decreased from ~284 $m^2\ g^{-1}$ (TiO_2) to ~146 $m^2\ g^{-1}$ (TiO_2/CIS), and further to ~41 $m^2\ g^{-1}$ for calcined TiO_2/CIS, while the total pore volume decreased from ~0.23 to ~0.13 $cm^3\ g^{-1}$, and to 0.001 $cm^3\ g^{-1}$ respectively. UV-Vis spectroscopy showed an enhanced visible-light absorption, especially in the vis-NIR range in TiO_2-CIS, while their photoluminescence (PL) analysis was carried out to investigate charge recombination dynamics. By coupling anatase/rutile TiO_2 and $CuInS_2$ QDs we aim to form a type-II and/or S-scheme heterojunction, to enhance solar energy utilization and photocatalytic performance [3]. CO_2 photoreduction is being performed in the liquid phase under simulated sunlight, with the liquid products analysed by gas chromatography.

Acknowledgement: Sara Venturi's work was supported by a PhD PNRR scholarship (MUR, D.M. n. 630/2024) partially funded by Hysytech s.r.l.

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FL28

Synthesis of Zeolitic imidazolate framework-8 (ZIF-8) in solvents alternative to DMF

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Zeolitic imidazolate frameworks (ZIFs) are a subclass of the well-known metal organic frameworks (MOFs), a new kind of crystalline porous materials which have gained an increasing interest among the scientific community for their extensive structural design possibilities. Among them, ZIF-8 stands out, consisting of tetrahedral units where each Zn ion coordinates four 2-methylimidazolate linkers, forming a three-dimensional sodalite-type topology. Due to their remarkable properties such as high crystallinity and porosity, large surface area and exceptional thermal and chemical stability, ZIF-8 are considered as attractive candidates for applications like gas storage and separation, catalysis and sensing. The properties of ZIF-8 are strongly influenced by synthesis parameters like temperature, pH, reaction time, solvent, reactants' molar ratio and concentration. In this respect, many efforts have been made to control the structural and morphological properties of ZIF-8 through the synthetic process. The solvothermal method using dimethylformamide (DMF) as solvent is commonly employed for the traditional synthesis of ZIF-8 [1]. However, since DMF is a toxic, fossil-based solvent that poses risks to human health and to the environment, developing new synthetic processes that use alternative solvents has become a primary goal in this field. In this context, glycerol carbonate (GlyC) has been successfully tested for the first time [2] as a green solvent for the synthesis of ZIF-8, showing a comparable performance to DMF but still showing high environmental impacts. To overcome this limitation, this work aims to explore the valorization of the waste obtained as by-product from the synthesis of GlyC, specifically the dimethyl carbonate-methanol mixture (DMC-MeOH), as an alternative solvent for the synthesis of ZIF-8. The latter involves $Zn(OAc)_2$ and 2-methylimidazole (Hmim) as precursors, in the presence of NaOH. Additionally, the synthesis of ZIF-8 is investigated using pure DMC, a highly recommended green solvent due to its non-toxicity and biodegradability (90% within 28 days) [3]. Various experimental conditions and synthesis parameters are being investigated to optimize the new proposed processes, in particular different reactants' concentrations as well as different temperatures, while keeping reaction time and reactants' molar ratio fixed. Finally, following the Green Chemistry principles, the potential of recycling the used solvents for further ZIF-8 synthesis is being evaluated to minimize the environmental impacts related to the process. Green metrics like E-factor and Process Mass Intensity (PMI) are being determined to quantify respectively the waste and the mass effectiveness of the reaction.

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FL29

Electroanalytical determination of cannabinoids in hashish samples for future implementations in electrochemical sensors

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Cannabis and its derivates (such as hashish) remains nowadays one of the most commonly used drugs of abuse in Europe, with 8,4% of young adults and adults reporting use in the last year [1]. Its psychotropic effects stem from Δ^9-tetrahydrocannabinol (Δ^9-THC). Recently, products with low Δ^9-THC levels but high cannabidiol (CBD) content have become available on the market, posing new challenges for cannabinoids detection and analysis. Our research group has been working for years on the development of innovative electrochemical sensors for the rapid detection of these analytes [2].

The construction features of SPEs (Screen Printed Electrodes) make them particularly suitable for their use in electrochemical sensors. For this reason, in this work, a specific type of SPEs modified with carbon black were used for the electrochemical determination of the cannabinoids content of real hashish samples. The extraction procedure of the samples and the instrumental parameters (15 mV/s potential scan rate with 50 mV pulse potential, 6 mV step potential, 0.1 s pulse time and 0.4 s interval time) used for the analyses were also optimized.

Using the same working conditions, standard solutions at different concentrations of the main cannabinoids present in the hashish extracts were analysed. The analysis of these standard solutions allowed for the construction of specific calibration curves as well as the application of the standard addition method to limit the matrix effect, ensuring the possibility to obtain a quantitative determination of the cannabinoids content in the real samples.

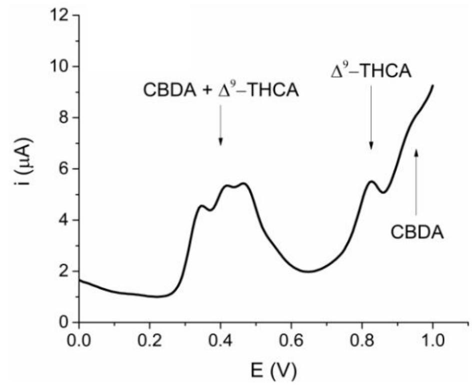

Figure 1: Example of a DPV signal recorded by applying our analysis procedure to a hashish extract. The arrows indicate the characteristic peaks of Δ^9-THCA and CBDA.

[1] https://www.euda.europa.eu/publications/european-drug-report/2025/cannabis_en

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FL30

Detecting circulating miRNA for next-generation liquid biopsy in breast cancer

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MicroRNAs (miRNAs), short single-stranded non-coding RNAs, have emerged as promising biomarkers in cancer diagnostics thanks to their stability and disease-specific expression. Their ability to reflect tumor heterogeneity makes them particularly suitable for liquid biopsy applications [1]. Concerning triple-negative breast cancer (TNBC), this aggressive and heterogeneous subtype is characterized by the deregulation of multiple miRNAs. Among them, miRNA-21 is consistently upregulated, and its overexpression has been strongly associated with poor prognosis, making it a valuable candidate for early diagnosis, risk stratification, and targeted therapies [2]. Despite their clinical relevance, conventional miRNA quantification methods are often complex, time-consuming, and require specialized personnel, which limits their accessibility in low-resource settings. To overcome these challenges, electrochemical point-of-care (POC) platforms, simple, rapid, and cost-effective, represent a promising alternative, minimizing matrix effects and exploiting low-cost, eco-friendly substrates [3]. In this work, miRNA-21 was selectively detected using a complementary DNA probe modified with methylene blue, serving as a redox mediator, immobilized on a gold nanoparticles (AuNPs)-functionalized, paper-based screen-printed electrode. Key experimental parameters and sensor's selectivity were carefully optimized, enabling reliable detection of miRNA-21 in both standard solutions and human serum. The platform demonstrated a limit of detection of 1.2 nM, a repeatability of approximately 8% and an excellent specificity. Sensitivity was further enhanced tenfold by integrating an external paper-based origami pre-concentration device, allowing detection down to the pM range. This research introduces a portable, rapid, and cost-effective diagnostic platform tailored for TNBC, enabling targeted molecular detection through minimally invasive testing. Its versatile, user-friendly design offers a practical foundation for accessible point-of-care testing, with significant potential for early, sensitive TNBC detection and personalized, precision treatment strategies.

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FL31

Synergistic use of nanomaterials and rice husk-derived silica for sustainable water purification

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Clean water scarcity is becoming an urgent health issue in many regions of the world, and Goal 6 of the UN's 2030 Agenda for Sustainable Development aims at halving the proportion of untreated wastewater and substantially increase recycling and safe reuse globally. Nanotechnology can provide effective solutions for sustainable water purification by integrating nanomaterials with bio-derived adsorbent material. Metal oxide nanoparticles such as zinc oxide (ZnO) and copper oxide (CuO) exhibit strong antimicrobial activity through mechanisms including ion release, oxidative stress, and membrane or DNA disruption [1-2].

On the other hand, rice husk, an abundant agricultural waste, can be converted into porous silica through acid leaching and calcination, providing a high-surface-area, low-cost adsorbent material [3].

The combination of rice husk-derived silica matrices and metal oxide nanoparticles provides multifunctional composites with enhanced adsorption properties and biocidal performances. This integrated approach represents a sustainable strategy toward next-generation water treatment technologies with the upcycling of agricultural byproducts, according to the principles of Green Chemistry.

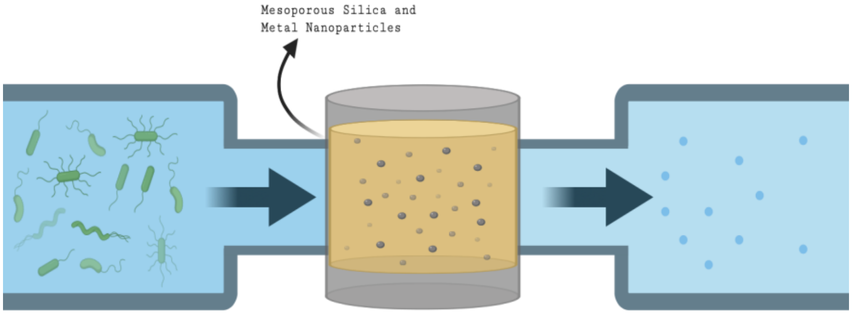

Figure 1: Schematic illustration of a water purification system.

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FL32

Development of T30175 G-quadruplex analogues as potential drug carriers

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In this study, we present an investigation on six analogues of anti-human immunodeficiency virus type 1 (HIV-1) integrase (IN) and antiproliferative aptamer T30175 (collectively referred to as INTB) [1], each incorporating 3′–3′ inversion of polarity sites and 2′-fluoro (2′-F) nucleotides as RNA analogues at various positions. These modifications were introduced to develop aptamers with enhanced thermal stability and improved nuclease resistance in serum compared to the original T30175 aptamer.

The physicochemical properties were characterized using a range of biophysical techniques, including circular dichroism (CD) spectroscopy, FRET melting assays, ISO-FRET assays, UV spectrophotometry (IDS and TDS), and nuclear magnetic resonance (NMR) spectroscopy. These analyses, complemented by polyacrylamide gel electrophoresis (PAGE), provided structural insights into the ability of the T30175 analogues to adopt G-quadruplex (G4) structures.

Furthermore, the binding affinity of these sequences for various G4 ligands with known antiproliferative activity (360A, PhenDC3, TMPyP4), and nucleolin (NCL), was evaluated using techniques like G4-Fid assay, Polyacrylamide Gel Electrophoresis (PAGE) and fluorescence spectroscopy. Preliminary results suggest that all aptamers effectively bind ligands, opening the way for the development of T30175 and its analogues as potential drug carriers.

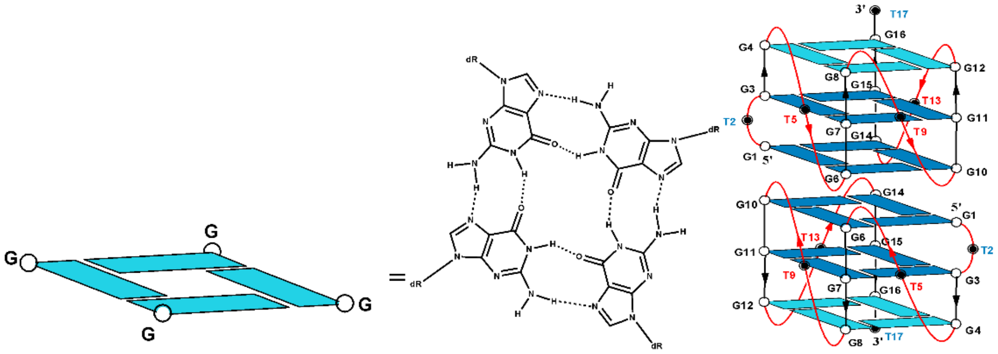

Figure 1: Schematic representation of a G-tetrad and the T30175 (INTB) G-quadruplex.

[1] Virgilio A, Amato T, Petraccone L, Esposito F, Grandi N, Tramontano E, Romero R, Haider S, Gomez-Monterrey I, Novellino E, Mayol L, Esposito V, Galeone A. Improvement of the activity of the anti-HIV-1 integrase aptamer T30175 by introducing a modified thymidine into the loops. Sci Rep. (2018).

FL33

Influence of synthesis conditions on the structure and electrochemical performance of Prussian White KMnHCF

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Owing to their 3D open frameworks, large interstitial sites, abundant redox active sites, low cost, and environmental benignity, Prussian Blue and its analogues (PBAs) have been attracting interest as highly promising cathode materials for Zn-based batteries, due to their ability to reversibly store zinc ions. Among the various PBAs, Prussian White potassium manganese hexacyanoferrate (KMnHCF, $K_xMn[Fe(CN)_6]1\text{-}y\square y\cdot nH_2O$) stands out for its high theoretical capacity, low cost, and environmental compatibility [1]. However, the practical performance of KMnHCF is limited by structural vacancies and interstitial water content, which (i) destabilizes the framework, (ii) reduce potassium content, and (iii) promotes Mn dissolution during cycling, all of which hinder the long-term cycling performance [2]. Since both defect concentration and water content are highly sensitive to synthesis conditions, the introduction of additives has been proposed as a strategy to tune nucleation and growth during KMnHCF synthesis via coprecipitation. Trisodium citrate dihydrate (Na3C6H5O7•2H2O) acts as a chelating agent that slows down the crystallization rate, thereby reducing lattice defects3. Polyvinylpyrrolidone (PVP), on the other hand, is known to suppress water incorporation and improve particle crystallinity by increasing steric hindrance and weakening electrostatic interactions between CN^- ligands and water molecules [3]. In this study, we investigate how citrate and PVP influence the final structure, composition and electrochemical performance of KMnHCF upon varying key synthesis parameters, including temperature (25 vs 80℃), stirring time, and atmospheric control (air vs. N2). By comparing additive-free KMnHCF (PW) with citrate-modified (PW^+) and citrate/PVP co-modified (PW^{++}) samples, we aim to correlate synthetic parameters with changes in particle morphology, alkali ion content, defect density, and water coordination. A combination of spectroscopic and analytical techniques (XDR, FTIR, Raman, TGA, SEM..) complemented by electrochemical methods (CV, GCPL, EIS) are employed to assess the effect of this structural modification on the electrochemical performance of the materials in laboratory-scale cells. This work offers critical insights into how synthesis-driven control of KMnHCF can be leveraged to optimize its performance in sustainable, aqueous Zn-based battery systems conceived for large-scale (seasonal) energy storage.

Acknowledgement: This study is supported by the MSCA-funded European Union project eNargiZinc (Grant Agreement No. 101120311) under the Horizon Europe Framework Programme.

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[3] Yan, C. et al. Electrochimica Acta 2020, 332, 135533

FL34

Phenothiazine–triarylamine small molecule hole transport materials for next-generation semi-transparent perovskite solar cells

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Perovskite Solar Cells (PSCs) exhibit remarkable tunability in their optoelectronic properties, enabling the development of wide band gap photo-absorbers that are well-suited for next-generation applications, including semi-transparent devices that can be seemly incorporated into building-integrated photovoltaics (BIPV) [1]. However, challenges in long-term stability and scalability hinder industrial adoption, requiring innovations across all device layers, with hole transport materials (HTMs) playing a crucial role for improving efficiency, stability, and durability. Phenothiazine (PTZ) is an attractive scaffold for developing novel hole transport materials (HTMs) due to its electron-rich core, low cost, and tunable redox properties. Its nonplanar geometry suppresses aggregation, while multiple functionalization sites enable precise tuning of electronic structure and energy levels. These features make PTZ-based frameworks highly promising candidates for efficient and stable HTMs in wide band gap and semi-transparent perovskite solar cells [2]. Herein, we report three novel small-molecule hole transport materials based on a phenothiazine–triarylamine cores, synthesized in a few moderate-to-high yielding steps. When integrated into $FAPbBr_3$-based semi-transparent perovskite solar cells, two candidates (SM1 and SM2) delivered power conversion efficiencies (PCE) comparable to, or even exceeding, the commercial benchmark poly(triarylamine) PTAA. In addition, their high light utilization efficiency (LUE) and outstanding bifaciality factor (BFF) highlight their potential as cost-effective and scalable HTMs for semi-transparent perovskite solar cells.

This work acknowledges support from Project CH4.0 under the MUR program "Dipartimenti di Eccellenza 2023-2027" (CUP: D13C22003520001), Spot-IT and JUMPINTOSPACE European Funded Projects.

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FL35

A rational design strategy for visible light-modulable dual-target AChE/MAO-B inhibitors

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The multifactorial nature of neurodegenerative disorders poses a significant challenge for traditional single-target therapies. A promising strategy involves the development of multitarget-directed ligands (MTDLs). Their integration with photopharmacology, which enables unprecedented spatiotemporal control over drug activity, could further improve the overall therapeutic approach [1]. Our research focuses on engineering molecular photoswitches with dual-inhibitory activity against acetylcholinesterase (AChE) and monoamine oxidase B (MAO-B).

Building on a previously studied donepezil-like scaffold (**1**) [2], which exhibited potent dual-target inhibition but required UV light for its photoisomerization, we aimed to shift the absorption spectrum towards the safer and more deeply penetrating visible light range. This objective was achieved through an isosteric replacement strategy, where the endocyclic methylene group of **1** was systematically substituted with heteroatoms (-O-, -S-, and -NH-).

This approach successfully tuned the electronic structure of the new analogues, inducing a pronounced bathochromic shift in the absorption spectra. Importantly, the photochemical characterization confirmed that the light-induced structural changes, vital for differential *E*/*Z* isomer activity in the parent compound, were maintained.

This work highlights a successful strategy for developing novel, visible-light-modulable MTDLs, paving the way for advanced light-controlled therapeutics with improved safety and precision for the treatment of neurodegenerative diseases.

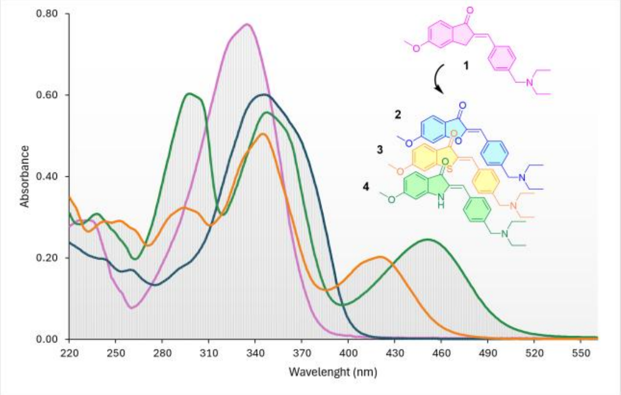

Figure 1. Color-coded UV-Vis absorption spectra of the studied compounds and their corresponding chemical structures.

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[1] Velema, W. A. et al., *J. Am. Chem. Soc.* 2014, 136, 6, 2178–2191.
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FL36

Catalyst-Free Synthesis of α-C-Glycoside Derivatives via Giese Reaction Driven by Photoactivated Electron Donor–Acceptor (EDA) Complexes

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Glycoproteins play a crucial role in numerous biological processes, including those associated with diseases and infections. Therefore, the development of glyco-amino acids and glycosyl conjugates has emerged as a promising strategy for elucidating biological pathways and discovering novel therapeutics. Here, we present a Hantzsch ester (HE)-induced glycosyl radical generation protocol from glycosyl iodides, leveraging an α-selective Giese-type reaction with electron-withdrawing olefins as a transition-metal-free synthetic approach to access C-glyco-amino acids and C-glycosyl conjugates. The proposed reaction mechanism, aligned with recent investigations of alkyl and aryl analogues, provides that radicals are generated through donor activation via a photoactivated electron donor-acceptor (EDA) complex with Hantzsch ester. This process is driven by halogen bonding, which facilitates electrostatic attraction and charge transfer, ultimately generating glycosyl radicals that undergo Giese-type addition reactions with suitable acceptors. We validate this approach with various acceptors to demonstrate its reproducibility and utility in accessing a library of highly valuable α-C-glycosyl conjugates.

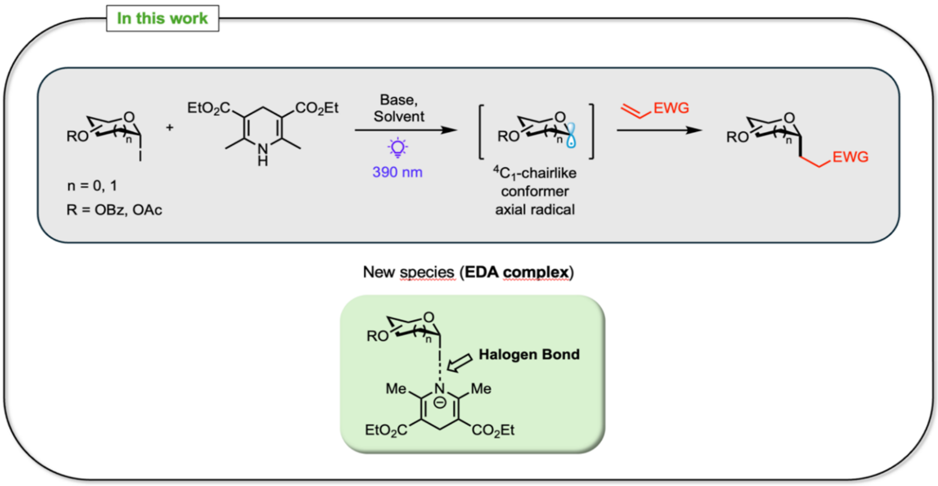

Figure 1: *Reaction investigated in this work.*

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FL37

Designing efficient photocatalysts for green solar-to-propellant conversion

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The simultaneous photocatalytic generation of hydrogen (H_2) and hydrogen peroxide (H_2O_2) from pure water is a challenging process, which requires materials with appropriate band-edge alignment and high stability under reaction conditions [1]. In the co-production scheme, H_2O_2 originates from the two-electron water oxidation reaction ($2e^-$ WOR) driven by photogenerated holes in the valence band, whereas H_2 is produced via the hydrogen evolution reaction (HER) at the conduction band. Achieving both pathways simultaneously relies on efficient charge carrier separation and suppression of electron–hole recombination. However, the decomposition of H_2O_2 on the catalysts' active sites, especially in the presence of transition metals, represents a major bottleneck for the overall efficiency [2].

In this study, we investigated a library of wide-bandgap semiconductors (Figure 1), including TiO_2, $BiVO_4$, SnO, WO_3, g-C_3N_4, and ZnO_2. Various TiO_2 and $BiVO_4$ morphologies and crystalline phases were synthesised and compared, while a commercial TiO_2 reference (Degussa P25) was modified by photodeposition of metal nanoparticles to promote charge separation through semiconductor–metal Schottky junctions. Photocatalytic tests were performed in a batch reactor under simulated solar light, with online GC analysis to quantify hydrogen evolution, alongside complementary assays to monitor H_2O_2 generation and degradation.

Preliminary results highlight the strong dependence of the photocatalytic response on crystal phase and surface morphology, as well as the beneficial effect of metal nanoparticle deposition on charge carrier dynamics. These findings provide fundamental insights into the rational design of photocatalysts for solar-to-chemical conversion in pure water systems, operating without sacrificial agents.

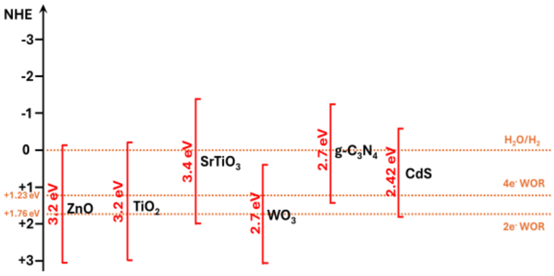

Figure 1: Band-edge positions of some semiconductor photocatalysts relative to the energy levels of various relevant photocatalytic processes

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FL38

Defect and morphology engineering of Strontium Titanium Oxide (STO) for enhanced photocatalytic water splitting

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The development of sustainable routes for high-added value chemical production to address energy crisis and climate change is a global priority. Photocatalysis offers a promising strategy, involving the harvesting of solar energy to drive uphill reactions such as water splitting and CO_2 reduction. In this context, solid inorganic semiconductors are particularly appealing due to their stability, recoverability, and reusability.

Strontium Titanium Oxide (STO) is a stable photocatalyst for water splitting, though its wide bandgap (3.2-3.3 eV) limits solar light exploitation. Defect engineering, especially lanthanide-nitrogen co-doping, has emerged as an effective route to extend light absorption [1].

A preliminary study employing a solvothermal synthesis produced flower-like STO exposing {110} facets [2], both lanthanide-doped and lanthanide-nitrogen co-doped, with different elements (Ce, Pr, Er, Yb). Tested for hydrogen photogeneration using a sacrificial agent, with and without Pt-NP co-catalyst, these samples showed high surface areas (up to ~190 $m^2\ g^{-1}$) and promising hydrogen generation rate (up to ~0.99 mmol $g^{-1}\ h^{-1}$); however, morphology inconsistencies and impurities complicated the interpretation. Recent optimization of the synthetic method has resolved these limitations, while current efforts also explore a complementary hydrothermal route to prepare cube-like STO [3] exposing {100} facets, guided by DoE approaches. The final aim is to assess hydrogen photogeneration with sacrificial agents, simultaneous photoproduction of hydrogen and hydrogen peroxide, and overall photocatalytic water splitting, employing lanthanide-doped and lanthanide-nitrogen co-doped STO across different dopants and both flower-like and cube-like morphologies.

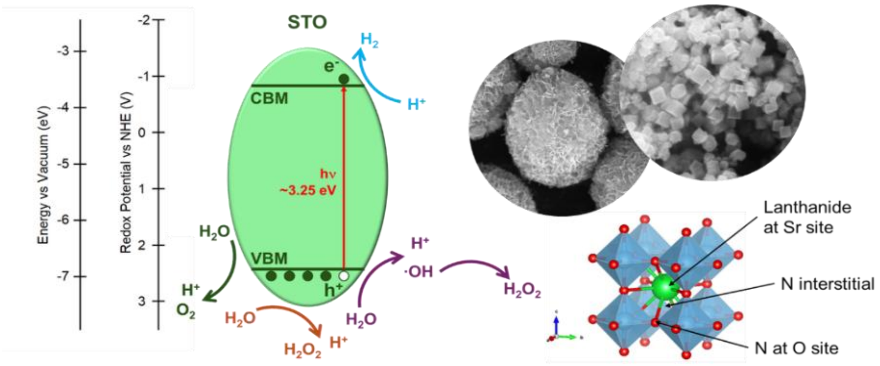

Figure 1: Approximate band alignment of STO with possible reactions at the band edges, FESEM images, and crystal structure with co-doping sites.

[1] W. Wei, Y. Dai, M. Guo, L. Yu, and B. Huang, *J. Phys. Chem. C* 113(33) (2009) 15046–15050.
[2] M. Zhou, J. Chen, Y. Zhang, M. Jiang, S. Xu, Q. Liang, and Z. Li, *J. Alloys Compd.* 817 (2019) 152796.
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FL39

Selective Semi-Hydrogenation Of Acetylene To Ethylene In Water Powered By A $CuInS_2$/ZnS QDs Photocatalyst

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Ethylene, one of the world's most important commodity chemicals, is the intermediate for ~60% of all plastics.[1] Ethylene is obtained by steam cracking and typically contains 0.5–2% of acetylene contaminant, which must be removed to produce polymer-grade ethylene.[2] Acetylene is typically removed by catalytic thermal hydrogenation at high temperature, with a precious metal (Pd)-based catalyst, and H_2 as the hydrogen source (**Figure 1a**).[2]

Recently, our group reported photocatalytic systems for the semi-hydrogenation of acetylene to ethylene.[3] These systems, while reducing acetylene with several advantages over the current state-of-the-art reaction, have two major drawbacks: (i) the need of an organic solvent and a hydrogenated organic as proton donor, and (ii) the need to work in tandem with a photosensitizer.[3]

This work describes the use of $CuInS_2$/ZnS QDs as an all-in-one photocatalysts for the semi-hydrogenation of acetylene to ethylene. Colloidal $CuInS_2$/ZnS QDs act as both catalyst and sensitizer reducing acetylene to ethylene with four main advantages over the current state-of-the-art reaction (**Figure 1b**): (i) operation with near 100% conversion of acetylene in an ethylene-rich gas feed while maintaining a selectivity ≥99.9% over ethane; (ii) the use of room temperature and visible-light to power the reaction instead of high temperatures and pressures; (iii) the use of water as proton source instead of H_2; (iv) the use of a noble metal free catalyst instead of a precious metal based one.

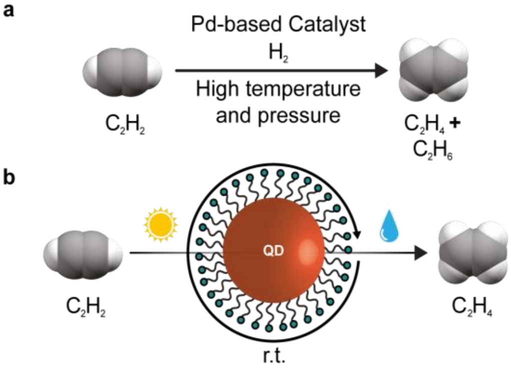

Figure 1. a) State-of-the-art process for the semi-hydrogenation of acetylene to ethylene. ***b)*** This work: ≥99.9% selective acetylene photoreduction to ethylene at room temperature using visible light and water as proton source.

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FL40

Aggregation-induced enhanced emission and photocatalysis with supramolecular polymers

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Aggregation can profoundly alter the excited-state properties of organic chromophores, yet its role in photocatalytic conversion of solar energy in chemical fuels is typically associated with charge delocalization or exciton transport in crystalline assemblies.[1,2,3] Here, we introduce aggregation-induced enhanced photocatalysis (AIEP), a supramolecular design principle in which aggregation activates photocatalysis by stabilizing localized singlet excited states. Using amphiphilic distyrylanthracene derivatives, we show that aggregation in water—triggered via concentration, charge screening, or counterion exchange—enhances fluorescence and enables light-driven transformations of solar energy into storable fuels, such as hydrogen (H_2) and hydrogen peroxide (H_2O_2). Enhanced reactivity correlates with increased excited-state population, underscoring the role of self-assembly in restricting intramolecular motion and suppressing unproductive non-radiative decay. The counterion dependence follows a reverse Hofmeister effect, with charge diffuse anions promoting aggregation, fluorescence, and function. Aggregated dyes also display enhanced photostability and recyclability compared to their molecular counterparts. Emission and catalytic activity are maximized in kinetically trapped aggregates, which outperform their thermodynamic counterparts, challenging conventional paradigm that photocatalysis is favored in extended assemblies. By achieving excited-state confinement and reactivity instead of charge delocalization, this work establishes supramolecular packing as a powerful strategy for designing photostable, emissive, and functional organic photocatalysts in water.

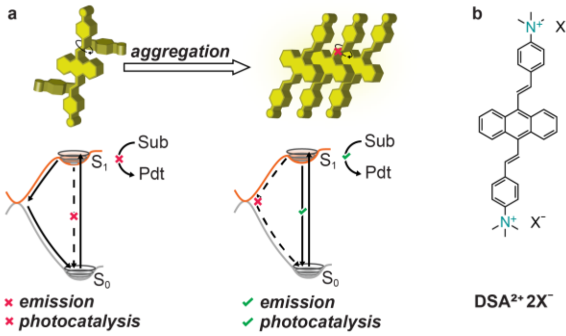

Figure 1: **a**, Overview of the dual aggregation-induced enhanced emission and photocatalysis with DSA amphiphiles (Sub = substrate; Pdt = product). **b**, Chemical structure of distyrylanthracene (DSA^{2+}) amphiphile, where X^- indicates the counteranion used.

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FL41

Polyphenols and nanocellulose extraction from spent coffee ground: a path to waste valorization

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Approximately 20 million tons of SCG are generated each year as a by-product of the brewing process, therefore the identification of potential applications for SCG is of great importance to reduce the environmental impact of the entire supply chain. Considering some source-dependent variations, generally dry SCG contains a non-negligible amount of bioactive compounds, including polyphenols and diterpenes (≈ 3-5%), within a consistent share of oils and lipids (≈ 20%). It also contains polysaccharides such as cellulose and hemicellulose (≈ 50%), lignin and proteins [1].

Following the extractions of the lipid, polyphenolic and diterpenic components, from SCG it is also possible to recover the cellulose-rich solid residue, which finds application in compounding or can be further processed to obtain functionalized nanocellulose.

In the present study, the optimization of sustainable extraction processes for the recovery of polyphenols is integrated with the extraction of functionalized nanocellulose as defined in the a recently licensed patent [2].

A laboratory-scale study was performed by testing different NADES (natural deep eutectic solvents) in thermal and microwave-assisted extraction of oils. Interesting results were observed regarding for the selective extraction of polyphenolic compounds in comparison with standard techniques such as Soxhlet organo-solvents extraction. After removing and recovering the lipidic, polyphenolic and diterpenic fractions, we proceeded with further valorizing the residue by bleaching the recovered solid and extracting the regioselectively functionalized nanocellulose by TEMPO-mediated oxidation.

The results support the potential of SCG as a valuable raw material within a biorefinery framework, promoting a circular economy approach and contributing to the sustainable development of waste-to-resource strategies.

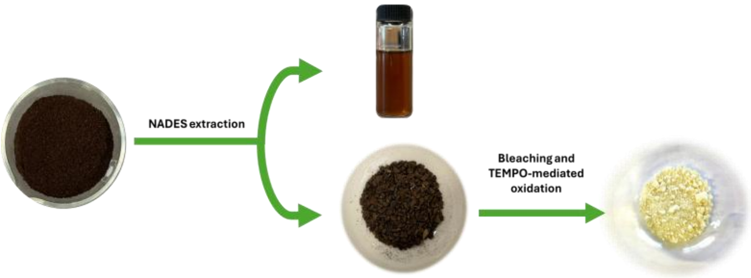

Figure 1: Valorization process scheme

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FL42

Grape pomace as an alternative source for the sustainable production of polyphenol-rich extracts

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The increasing demand of agro-industrial products worldwide is making their by-products a serious problem affecting the global ecosystem and environment because of their accumulation and disposal [1]. Being a rich source of polyphenols, grape pomace has already proven in our previous, recent paper, through HPLC-DAD analysis, antioxidant and antimicrobial assays, to be a precious secondary raw material to have an alternative usage to assist human health [1]. In this follow-up work, seventeen different varieties of grape pomaces, collected from Apulia (Italy), have been used to perform the solid-liquid extractions with the previously identified best Deep Eutectic Solvents (DESs). These media represent an alternative and ecological solution to classic solvents and can be considered edible for animals and/or humans [1]. Chemical analyses of the extracts were performed at HPLC-DAD, using the already published optimized method [1], to investigate the presence of fourteen selected phenolic compounds. Then, Sangiovese and Merlot grape pomaces' varieties, extracted with Betaine/Lactic Acid (1:4 mol/mol + 40% H_2O; Bet/LA) and Choline Chloride/Ascorbic Acid (2:1 mol/mol + 40% H_2O; CC/AA), were selected for a further analysis at LC-QTOF-MS. The presence of sixty-two polyphenols was assessed with extracting yields around three times higher or more for Bet/LA compared to CC/AA Acid DES. Agar diffusion antimicrobial assays contributed to confirm these results showing a much less qualitative efficacy for Choline Chloride-based DES extracts, especially against pathogenic fungi. Then, in vitro digestion experiment was carried out on freeze-dried Bet/LA DES extracts both from Sangiovese and Merlot grape pomaces to deepen differences in composition and bioactivity in each studied phase. The obtained results will be discussed for a possible application of these products as food and/or feed supplements.

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FL43

Turning blue crab shell into a resource

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Sustainability and environmentally friendly practices have become urgent imperatives in the face of escalating environmental challenges. They are key drivers of innovation in recycling technologies and resource recovery strategies, encouraging a rethinking of our consumption patterns and waste generation. In this context, waste can be redefined not as burden, but as valuable source of functional molecules connecting ecological responsibility and economic potential [1]. Callinectes sapidus, native to the Atlantic coasts of Americas, is an invasive species known for its adaptability, high reproduction rate and aggressive behavior. Its characteristics allowed it to spread to new coastal habitats, including Mediterranean Sea, making its management essential [2]. The aim of this study is to valorize molecules naturally present in Blue crab's carapace, such as astaxanthin, using environmentally friendly extractions, in order to manage the resulting waste after crab's meat consumption, which is considered one of the most tasting in the world. Astaxanthin is a xanthophyll, member of the carotenoid family, and exhibit various biological activities. These include, among the others, antioxidant effects, lipid peroxidation, anti-inflammatory properties, cardiovascular disease prevention and so on [3]. Blue crab is primary desiccated, grounded, collected in vacuum-sealed food bags and stored in freezer. Blue crab powder is put in contact with NADES (Natural Deep Eutectic Solvents) under magnetic stirring and the astaxanthin enriched extract can be analyzed through UV-Vis spectroscopy and other approaches. In this preliminary analysis Astaxanthin is successfully extracted from blue crab carapace. These results align with the principles of the circular economy, not only by using waste materials but also employing green solvents that are either food grade or potentially reusable.

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FL44

Cannabizetol, a novel cannabinoid: chemical synthesis, anti-inflammatory activity and extraction from *Cannabis sativa* L.

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Methylene-bridged dimers represent a class of over 130 natural products which is gaining increasing attention due to their structural diversity and biological activity [1]. *Cannabis sativa* is a well-known source of bioactive principles, including over 150 phytocannabinoids. While the biological activity of "major cannabinoids" (as Δ^9-THC, CBD, CBG and CBC) is well explored, the study about minor cannabinoids, present in plants as traces, still remains limited, mostly due to isolation issues [2]. Recent efforts have led to the discovery of two methylene-bridged dimers: cannabisol and cannabitwinol, respectively homodimers of Δ^9-THC and CBD [1]. In this work [3], we report the discovery of the third member of this class, cannabizetol (CBGD, Fig.1), homodimer of CBG. We combined the chemical synthesis of CBGD with its identification in *Cannabis sativa* extracts. The synthesized compound was fully chemically characterized and used as a reference to identify and isolate its natural counterpart. Cannabitwinol and CBGD were evaluated in HaCaT keratinocytes, demonstrating significant anti-inflammatory activity, including inhibition of NF-κB signaling and IL-8 secretion, with CBGD showing higher biological activity. Encouraged by these results, we developed a one-step flow synthesis starting from CBG, representing the first continuous approach to methylene-bridged dimers preparation.

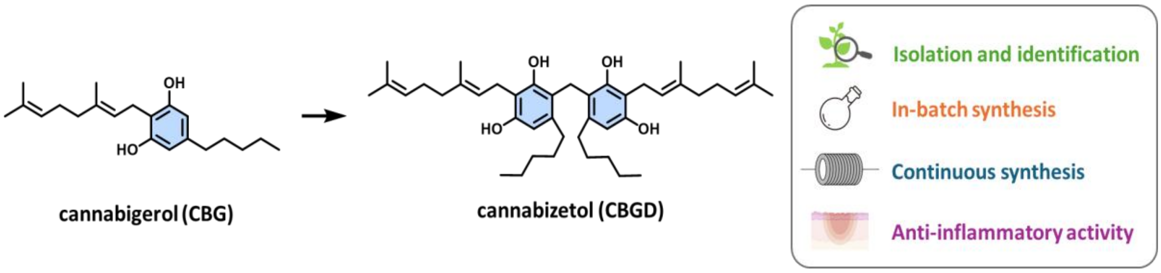

Figure 1: Structures of CBG and its homodimer CBGD

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FL45

Real-time monitoring of VOCs employing PTR-ToF-MS for shelf-life assessment in *Agaricus bisporus*

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Agaricus bisporus (white button mushrooms) is the most widely cultivated edible mushroom worldwide because of its good texture, unique flavor, sensory qualities, and nutritional characteristics such as high-protein and low-fat content [1].

In this study, Proton Transfer Reaction-Time-of-Flight Mass Spectrometry (PTR-ToF-MS) was used to monitor volatile organic compounds (VOCs) using both non-destructive (whole mushrooms) and destructive samplings. Mushrooms were stored under different conditions (4°C, 20°C and a stress scenario involving cold chain breaks every two days for six hours). In addition, a smart, reusable, recyclable and stackable packaging system (StoreBox) was tested for its potential in reducing food loss and quality degradation during postharvest storage. Dynamic headspace (non-destructive) represented the aroma of intact mushrooms during storage. On the other hand, static headspace (destructive) released intracellular volatiles and enzymatic products, revealing the potential VOC reservoir.

VOCs such as ethanol, acetaldehyde, methanethiol, and hexanal are key spoilage markers in *Agaricus bisporus* [2]. In our work, the mentioned compounds were consistently detected in both dynamic and static headspace datasets. Particularly, ethanol (*m/z 47.049*) and acetaldehyde *(m/z 43.018*) showed a strong increasing trend over time in both packaging (STD and SB). The concentration of both compounds increased moderately under refrigeration compared to the stress condition after 15 days. On the other hand, the ambient temperature led to a much stronger increase in their concentrations.

Notably, static headspace data revealed VOC profiles parallel to dynamic headspace data and compositionally richer trends. Also, compared to SB samples these trends were more pronounced in samples from STD packaging, showing superior capability of SB packaging to preserve the mushrooms.

Overall, according to the findings, the combination of SB packaging and refrigeration can extend shelf life, preserve volatile integrity, and reduce postharvest losses in Agaricus bisporus distribution chains. This work supports the application of VOC fingerprinting as a powerful tool for monitoring freshness and highlights the potential of reusable, non-invasive packaging innovations in sustainable cold chain logistics.

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FL46

New butyric acid-releasing glucosamine derivatives for the treatment of inflammatory-based diseases

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Butyric acid (BA), a short-chain fatty acid naturally found in common foods, has been shown to be a potent modulator of various intestinal and extra-intestinal functions, playing a crucial role in controlling inflammation and pain. However, dietary intake of BA is often insufficient to promote optimal intestinal health and fully harness its numerous physiological and pharmacological benefits. Despite its potential, the clinical application of BA is limited due to its unfavorable physicochemical properties and unpleasant organoleptic characteristics, such as taste and odor. To meet the growing demand for BA derivatives, the prodrug approach, which involves chemically modifying a parent drug molecule to optimize its physicochemical and pharmacological properties, could represent an effective strategy in medicinal chemistry. The application of this strategy to synthesize new BA derivatives has led to improvements in pharmacokinetic properties, maintained a good atoxicity profile, and allowed further exploration of the role of these derivatives in pain treatment, particularly in nociception modulation [1-2].

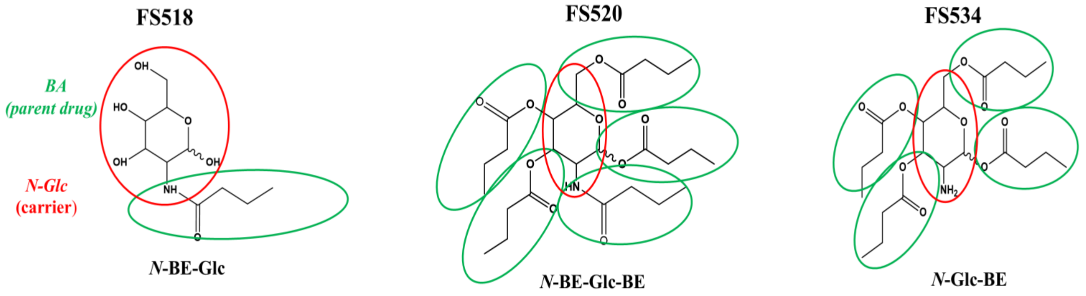

Figure 1: Chemical structure of new BA derivatives

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FL47

BREAST “Breast canceR Enhanced AI Supported Therapy”: AI-based machine learning algorithms for triple-negative breast cancer personalized treatment

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Triple Negative Breast Cancer (TNBC), defined by the absence of Estrogen Receptor (ER), Progesterone Receptor (PR), and ERythroBlastic oncogene B (ERBB2) expression, represents one of the most aggressive Breast Cancer (BC) subtypes. Its resistance to conventional therapies and high invasiveness present clinical challenges. In the absence of a definitive standard treatment, leveraging Artificial Intelligence (AI) holds promise for advancing pharmaceutical research. Here, we present the development of the BREAST model (Figure 1), designed to predict personalized anticancer therapies for TNBC patients based on their proteomic profiles. Our approach utilized data from The Cancer Genome Atlas (TCGA) [2] and The Cancer Proteome Atlas (TCPA) [3], including genomic, proteomic, and clinical data, to correlate omics signatures with treatment outcomes. A key effort was devoted to cross-matching datasets at the patient level, ensuring that each patient ID was accurately aligned across all dimensions. The methodology employed a variety of ML techniques such as Random Forest (RF), Support Vector Machine (SVM), Neural Networks (NN), Gradient Boosting (GB) and a 5-fold cross-validation to assess their performance using metrics such as Area Under the Curve (AUC) and the 1% Enrichment Factor (1%EF). Data analysis showed that the models achieved AUC values of 0.980 ± 0.017 (SVM), 0.998 ± 0.002 (RF), 0.989 ± 0.009 (XGBoost), and 0.984 ± 0.011 (LR). Feature importance analysis highlighted biologically relevant proteins known to be involved in TNBC, confirming the biological plausibility of the model. These findings pave the way for the future application of the BREAST model in hospital settings, with the ultimate goal of supporting oncologists in selecting personalized therapies for TNBC patients.

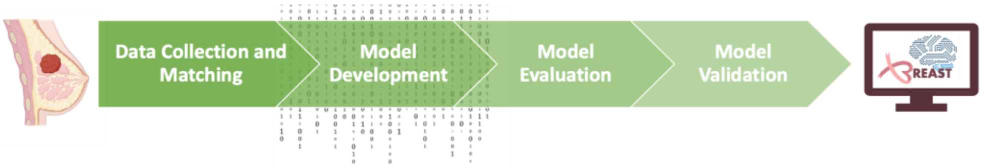

Figure 1: BREAST model pipeline: data collection, learning, and validation.

Acknowledgments*:* Alessia Bono was supported by Fondazione Umberto Veronesi.

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FL48

Structural determinants underlying the supramolecular binding between carborane and proteins in water

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Carboranes are abiotic clusters composed of boron, carbon, and hydrogen atoms that exhibit exceptional chemical and biological stability, making them promising scaffolds in medicinal chemistry. Their applications have been extensively explored in boron neutron capture therapy (BNCT), but their hydrophobicity hinders their direct in vivo administration [1]. Proteins, acting as "Trojan horses" [2], can be used as supramolecular hosts for carborane in physiological environments.

Here, we report the first complete characterization in solution of the interaction between carborane and a model protein, lysozyme (LSZ). Experimental data demonstrate that carborane forms a stable 1:1 complex with LSZ, which maintains its structure and monomeric state upon interaction. NMR chemical shift perturbations, corroborated by computational studies, reveal that the carborane cage fits precisely into a well-defined hydrophobic pocket: the binding is primarily driven by van der Waals and hydrophobic interactions, complemented by "classical hydrogen bonding" and "non-standard dihydrogen bonding". The formation of the complex leads to a partial inhibition of enzymatic activity (~38%), consistent with steric interference at the active site of the protein.

These findings highlight the capability of carborane to engage in selective, non-disruptive protein interactions through its unique chemical features. The implications extend beyond drug development to areas such as protein tagging, delivery strategies for BNCT, and the rational design of carborane-based inhibitors.

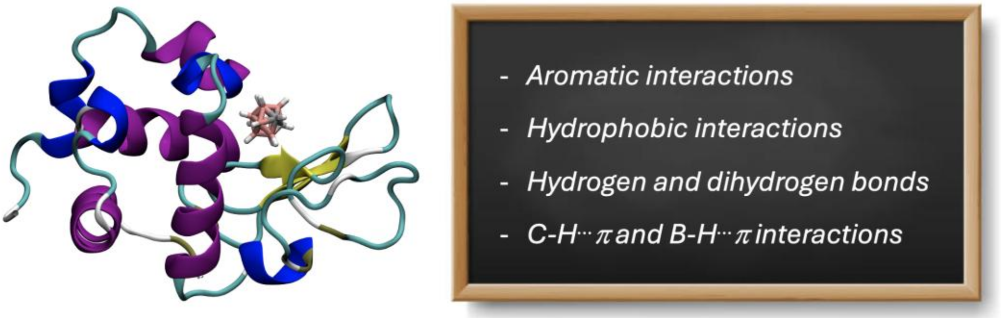

Figure 1: Binding of carborane in the lysozyme substrate binding pocket.

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FL49

Fluorescent BN-CDs for light-emitting devices

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Boron- and nitrogen-doped carbon dots (BN-CDs) are luminescent nanomaterials that are promising for optoelectronic devices such as light-emitting cells (LECs) and diodes (LEDs) due to their photoluminescent properties, non-toxicity and relative ease of production. The major limitation of their application in solid-state devices is aggregation-caused quenching [1]. The strong interaction between crystalline C-cores leads to a part or complete loss of fluorescence during the transition to the powder state. In contrast, amorphous or partially crystalline BN-CDs nanodots with functional groups on the surface could facilitate the effective separation of sp^2 domains allowing for bright solid-state fluorescence [2].

For this purpose, we prepared amorphous BN-CDs (Figure 1a) using a water-based microwave synthesis from a mixture of boric acid, urea, and citric acid (B, N, C source, respectively). The purified nanodots fraction showed a bright, excitation-independent blue-emission in solution (440 nm, PLQY 42%), as shown in Figure 1b. To preserve fluorescence in the solid state, the BN-CDs were introduced into the polymeric hydrophilic matrix [3]. The efficient energy transfer from the polymeric host to the guest (BN-CDs) resulted in good performance of the light-emitting device: maximum luminance of 40 cd/m^2, and stability of a few hours. Moreover, the interaction of the surface of BN-CDs with other components of the active layer led to the white emission of the final LEC device, as shown in Figure 1c, characterized by x/y CIE coordinates of 0.30/0.35, correlated color temperature of 6,795 K, and color rendering index of 87 [3].

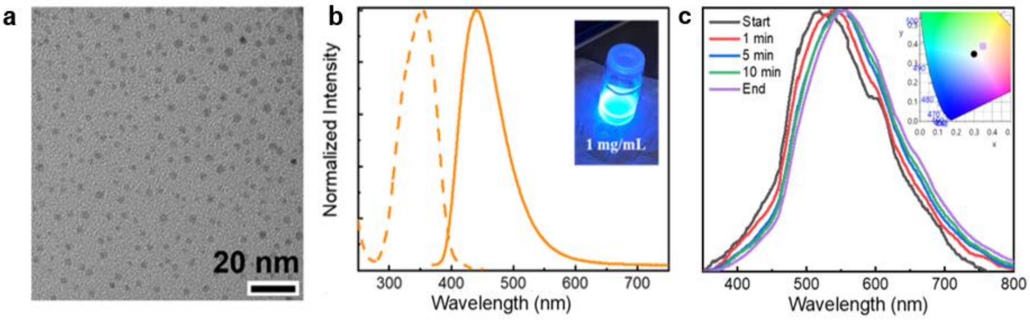

Figure 1: (a) TEM image of BN-CDs; (b) Normalized excitation (dashed line) and emission (solid line) spectra of BN-CDs in aqueous solution (1mg/ml); (c) EL spectrum and x/y CIE color coordinates of BN-CDs-based white light-emitting LEC [3].

Acknowledgements: This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 956923 – StiBNite.

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FL50

Exploring activated ester warheads as covalent fragments with dual antiviral and anticancer applications

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Covalent selective inhibition has emerged as a powerful strategy in medicinal chemistry, enabling the development of potent and targeted therapeutics. Covalent inhibitors typically consist of a reactive warhead and a recognition moiety (driver region) [1]. Focusing initially on the warhead as a modular fragment allows assessment of its intrinsic reactivity and stability before elaborating the molecule to optimize target engagement. Fragment-Based Drug Discovery (FBDD) provides an ideal framework for this approach, facilitating the systematic exploration of small reactive fragments [2]. Within this strategy, our aim was to develop a library of activated ester fragments, given their demonstrated biological activities and high selective reactivity toward cysteine and lysine residues in key disease-related proteins [3].

The designed fragments were synthesized via efficient one-pot procedures and fully characterized for their physicochemical and drug-like properties. They were subsequently evaluated through biochemical assays on viral proteases (SARS-CoV-2 Mpro) and phenotypic assays in tumor cell lines. Several derivatives inhibited viral proteases with micromolar affinity, while others selectively impaired proliferation of melanoma (A-375) cells in vitro, with IC_{50} values below 2 µM. In melanoma cells, these compounds induced apoptosis, cell-cycle arrest, mitochondrial dysfunction, and increased ROS production, while sparing non-tumorigenic cells. For the most promising derivatives, stability in physiological media and covalent reactivity toward nucleophilic residues were confirmed in acellular conditions.

Overall, these findings highlight the proposed esters as promising covalent fragments combining antiviral and anticancer activities, providing a modular starting point for further structural refinement and the design of more complex therapeutic candidates.

Acknowledgments*:* This work was supported by SiciliAn MicronanOTecH Research And Innovation Center "SAMOTHRACE" (MUR, PNRR-M4C2, ECS_00000022), spoke 3 -Università degli Studi di Palermo "S2-COMMs – Micro and Nanotechnologies for Smart & Sustainable Communities" (CUP B73C22000810001).

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FL51

Novel Benzyloxy-Substituted 2-Phenylbenzimidazoles: A Sustainable Approach to Develop Elastase Inhibitors

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Human skin elasticity and stability rely on extracellular matrix proteins such as collagen and elastin. Elastase 1, a serine protease expressed in keratinocytes, contributes to the proteolytic degradation of elastin, and its overactivity is linked to skin aging and disorders including psoriasis and dermatitis [1]. Selective elastase inhibitors therefore hold promise as therapeutic agents in both dermatology and cosmetology.

Recently, a series of *N*-[(3,5-dimethylphenyl)methyl]-1*H*-benzimidazole derivatives was identified by us [2] as inhibitors toward porcine pancreatic elastase (PPE), that is widely employed as a surrogate model for preliminary biochemical evaluation. Guided by *in silico* and experimental structural insights, we rationally designed a novel series of *N¹*-benzyloxy-2-phenylbenzimidazoles aimed at retaining PPE inhibitory activity while enhancing synthetic efficiency and sustainability.

Systematic substitutions at the 5- and 6-positions of the benzimidazole core, along with modifications of the N^1-benzyloxy and 2-phenyl moieties, were introduced to collect new structure–activity relationship (SAR) insights into PPE inhibition. Several compounds displayed anti-elastase activity, supporting the relevance of this chemical class as a viable alternative to the well-known chemotypes acting as irreversible inhibitors. Molecular docking (Figure 1) supported the SAR findings, highlighting hydrophobic and aromatic interactions as key determinants of PPE inhibition.

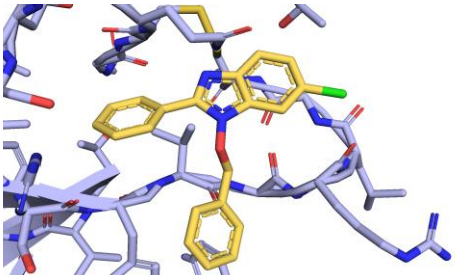

Figure 1: Plausible binding pose in the cavity of PPE.

This research was supported by the Italian Ministry of University and Research (MUR) grants assigned to Giovanna Pitasi (CUP: J44D22000960009) and Francesca Mancuso (CUP: J43C25000230006).

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FL52

Synthesis and formulation of estrogenic soft drugs

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Estrogens are steroid hormones with multiple biological activities, including a relevant role in wound healing. To mitigate their systemic effects, active molecules can be converted into soft drugs, which are active upon administration but rapidly inactivated by metabolism, thus enabling topical action only. In the first part of my project, I established a more efficient and sustainable synthetic route for the preparation of estrogenic soft drugs, avoiding functional group protections and implementing one-pot methodologies. This was complemented by the development of a dermal nanovesicular carrier. Liposomes were selected for their ability to enhance drug accumulation at the target site, as well as for their biocompatibility and non-toxicity. In our laboratory, two series of estrogenic soft drugs with hydrolysable ester group have been synthesized and, among all, **1**[1] and **2**[2] (Figure 1) resulted the most promising. In this work, we present preliminary studies on inclusion of **1** and **2** in liposomes and transfersomes. Transfersomes have a more flexible structure than liposomes thus enabling penetration through the epidermis. Several nanovesicular carriers [3] have been prepared using phosphocoline (dipalmitoylphosphatidylcholine, DPPC, or dimyristoylphosphatidylcholine, DMPC) as the main component in mixture with the estrogen derivative (**1** or **2**) and/or sodium cholate, the latter as the edge activator. Physicochemical properties were analyzed by DLS/DELS. After assessing stability, entrapment efficiency was evaluated to quantify drug incorporation and release. Drug release studies were carried out up to 24 h using UV spectrophotometry.

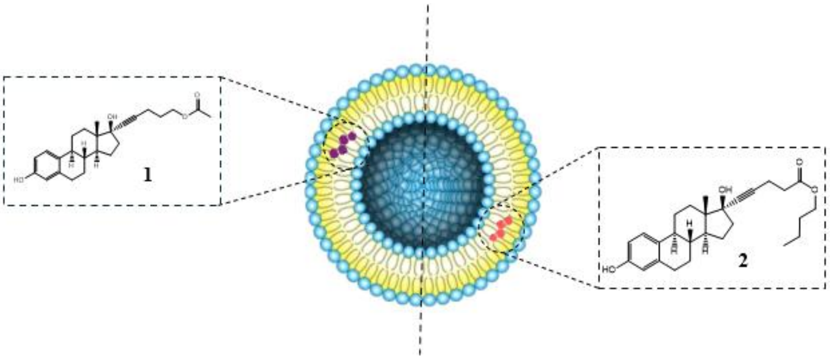

Figure 1: liposomes of estrogenic soft-drugs

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FL53

Computational design and evaluation of novel GPR84 PET tracers targeting neurodegenerative diseases

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Neurological diseases, such as multiple sclerosis (MS), Alzheimer's disease (AD) and Parkinson's disease (PD), represent a broad class of disorders characterized by chronic innate immune-mediated activation affecting the central nervous system (CNS). G-protein-coupled receptor 84 (**GPR84**), a transmembrane medium-chain fatty acid receptor, was shown to be expressed on the surface of immune cells (neutrophils, monocytes, and macrophages) [1] and to be upregulated under pro-inflammatory conditions. Therefore, GPR84 represents a novel and promising sensor of maladaptive innate immune responses for positron emission tomography (PET) imaging strategies as well as a potential therapeutic target [1].

Among GPR84 antagonists, one of the most studied classes contains a dihydropyrimido isoquinoline-2,4-dione core, with GLPG1205 advancing to first-in-human clinical trials [2]. Starting from GLPG1205 scaffold and introducing suitable structural modifications, our research group generated a first-in-class **^{18}F-MGX-110S** radiotracer, a highly promising tracer that detects proinflammatory immune responses in human cells and mouse models of systemic inflammation [3]. In order to generate a novel class of potential GPR84 antagonists and specific tracers, computational chemistry methods were implemented using a ligand-based approach.

First, we carried out the flexible alignment of the most potent known allosteric antagonists, followed by the generation of a pharmacophore model, which was then used to screen our in-house database, finding all the molecules that fitted the model. Subsequently, the cryo-EM structure of GPR84 was downloaded and prepared for docking, finding the most probable binding site. Molecular Dynamics (MD) simulations were optimized and performed, in the presence of a phospholipid bilayer (explicit membrane). Finally, six compounds were identified as potentially active against our target and biochemically and biologically evaluated from our collaborators at Stanford University.

In the future and basing on the results obtained with the first selected compounds, we will select other compounds and further decorate the most promising ones, to identify a lead molecule and develop a GPR84 highly selective compound with efficient brain uptake and minimal toxicity.

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[3] Unpublished results.

FL54

Pseudomonas aeruginosa Quorum Sensing systems as drug targets: design of new tools aimed at inhibiting biofilm formation

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Pseudomonas aeruginosa is a critical priority pathogen known for its multidrug resistance and its ability to form biofilms that contribute to persistent and hard-to-treat infections [1]. Biofilms are structured communities of bacteria enclosed in a self-produced polymeric matrix that protects them from antibiotics and the host immune response, playing a major role in the chronicity of infections, particularly in the lungs [1]. A key element in the pathogenicity of *P. aeruginosa* is the quorum sensing (QS) system, which coordinates the expression of virulence factors and regulates biofilm development [2]. Among QS regulators, the transcriptional factor PqsR (also known as MvfR) plays a central role. Activated by alkylquinolone signals such as PQS and HHQ, PqsR controls the expression of genes involved in virulence, iron acquisition, and critically, the formation and maturation of biofilms [3]. Due to its pivotal regulatory function, PqsR is considered an attractive anti-virulence target. PqsR inhibition reduces pathogenicity without affecting bacterial growth, thereby limiting resistance development and representing a promising strategy to disrupt QS, biofilm formation, and virulence in *P. aeruginosa* [2]. In this context, our research group previously published a series of quinazolinone-based small molecules capable of modulating PqsR activity, impairing both biofilm formation and virulence factors production. We subsequently optimized the most active compound of the series by modifying its terminal aromatic moieties to enhance both hydrophobic and hydrophilic interactions with the target protein. Several derivatives exhibited potency in the low micromolar range. Guided by structure–activity relationship (SAR) studies, the design and synthesis of new compounds based on a novel scaffold will be presented.

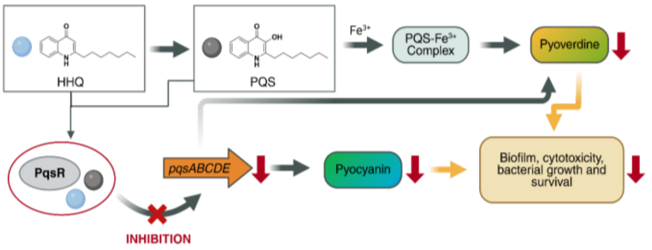

Figure 1: PqsR inhibition.

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FL55

Design and development of nucleophile-electrophile adducts based on cannabinoids as anti-inflammatory and antioxidant agents

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Chronic inflammation and oxidative stress are often referred to as "the causes of all diseases" and are largely mediated by the NF-κB (Nuclear Factor Kappa-Light-Chain-Enhancer of Activated B Cells)/Nrf2 (Nuclear Factor Erythroid 2-Related Factor 2-Kelch-Like ECH-Associated Protein 1) pathway. Phytocannabinoids, secondary metabolites of *Cannabis sativa L.*, act as NF-κB inhibitors and Nrf2 activators and thus represent appealing anti-inflammatory and antioxidant compounds [1]. However, their use is limited by significant pharmacokinetic challenges. This study focuses on cannabinoquinones [2]—oxidative products of phytocannabinoids—specifically those derived from non-psychotropic compounds. In particular, we aim to exploit the high electrophilic reactivity of cannabinoquinones to generate novel adducts with nucleophiles such as polar amino acids (AAs) or their biological derivatives, potentially leading to compounds with improved solubility and synergistic effects (Figure 1).

The new binary adducts will be tested in cell lines carrying gene reporters for NF-κB and Nrf2 to investigate the therapeutic potential, particularly the anti-inflammatory and antioxidant effects.

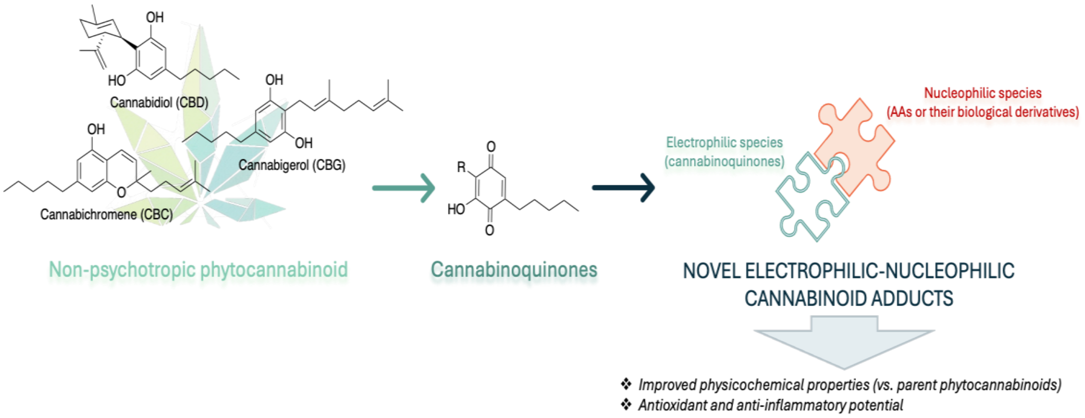

Figure 1: Design of bioactive adducts from cannabinoquinones.

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FL56

Targeting trypanothione reductase: Exploring the potential of 5-nitro-tiophene-based inhibitors

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Leishmania infections remain a significant global health issue, afflicting neglected populations mainly distributed in Africa, Asia and Latin America [1]. These protozoa are transmitted through the bite of female phlebotomine sandfly. The insect injects the infective, promastigote forms of the parasite, which subsequently are taken up by macrophages and proliferate intracellularly as amastigotes, ultimately leading to severe complications, the most lethal of them being visceral leishmaniasis, which affects key organs, causing splenomegaly, hepatomegaly, and serious gastrointestinal symptoms [2]. The treatment of Leishmania infections is often complicated by the lack of available vaccines and limited therapeutic options, rising drug resistance, with most of treatments being highly toxic to the host [3]. Targeting *Leishmania spp*., inhibition of the enzyme trypanothione reductase (TR) is a promising strategy to disrupt the trypanothione metabolism unique to the parasite and shared by all trypanosomatids, minimizing host toxicity [3]. Among the drug targets explored in this field, it has been demonstrated that pentavalent antimonials affect the TR activity, which is essential for survival of Leishmania parasite inside the macrophages. However, they have a low therapeutic window [3]. Our recent advances have led to the identification and development of novel 5-nitro-thiophene based inhibitors [3]. Following the established pharmacophore of TR inhibitors, the design of a new library of inhibitors, the optimization of the synthetic pathway for their preparation and analysis of the main structure-activity relationships derivated by their biological investigation will be here presented.

General pharmacophore of LiTR inhibitors

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FL57

Targeted Degradation of Translational Regulators in the Progression from MASLD to Hepatocellular Carcinoma

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Recent research has identified eIF6, a translation initiation factor that operates downstream of the insulin pathway, as a potential drug target. It acts as an anti-association factor, preventing the premature binding of the 60S and 40S subunits of eukaryotic ribosomes. Levels of eIF6 have been demonstrated to rise during the progression from Metabolic dysfunction-Associated Steatotic Liver Disease (MASLD) to Hepatocellular Carcinoma (HCC), one of the most lethal forms of cancer. It has also been demonstrated that an *in vivo* genetic depletion of eIF6 has resulted in a significant reduction of lipid accumulation in the liver, with an associated increase of fatty acid oxidation [1].

In light of these observations, the modulation of eIF6 activity emerges as a potential effective strategy to prevent the progression of MASLD to HCC, as well as for the treatment of existing HCC [2].

In order to validate this hypothesis, several putative eIF6 binders were identified through computational studies. The most promising candidates were then subjected to microscale thermophoresis binding affinity assays, which confirmed their ability to bind the translation factor in the low micro and nanomolar range. Consequently, a library of selective eIF6 degraders was developed by leveraging the molecular scaffolds of the top binders identified, employing emerging strategies such as Proteolysis Targeting Chimeras (PROTACs) and Hydrophobic Tags (HyTs). These innovative approaches enable the targeted degradation of a protein of interest by exploiting the ubiquitin-proteasome system or by mimicking a partially denatured or misfolded state of the protein and consequently leading protein's degradation through the proteasome pathway.

We are currently developing the first selective eIF6 degraders, whose design, synthesis, and characterization will be detailed and discussed.

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Poster presentations

POS01 – Allevi Dario (UniMI)

POS02 – Amaddio Corinne (UniMI)

POS03 – Bononi Giulia (UniPI)

POS04 – Bosetti Emanuele (UniBO)

POS05 – Boutagou Kawter (SNS)

POS06 – Caccia Aziza (UniMI)

POS07 – Caporale Marilena (UniBAS)

POS08 – Cartamina Emanuele (UNIINSUBRIA

POS09 – Castiglione Davide (UniTO)

POS10 – Cavinato Luca Maria (UniTO)

POS11 – Ceriani Federica (PoliMI)

POS12 – Cosenza Chiara (UniSI)

POS13 – Curia Arianna (PoliMI)

POS14 – D’Alessandro Eleonora (Campus Biomedico Roma)

POS15 – Doardo Matilde (UniPD)

POS16 – Fanciullacci Giorgia (UniFI)

POS17 – Fusto Letizia Maria (UniCT)

POS18 – Giammarino Francesca (UniSA)

POS19 – Grande Tommaso (UniInsubria)

POS20 – Gritti Alessandra (UniMI)

POS21 – Iennaco Alessia (PoliBA)

POS22 – Maccarino Lorenzo (UniUPO)

POS23 – Maiorana Leonardo (UniMI)

POS24 – Manca Gabriele (UniPG)

POS25 – Marotta Angela

POS26 – Martinini Samuel (UniBO)

POS27 – Massaro Arianna (UniNA)

POS28 – Meraviglia Silvia (UNIMI)

POS29 – Migliano Francesco (UNIMI)

POS30 – Milia Manuela (UNICT)

POS31 – Mori Leonardo

POS32 – Nardi Alberto

POS33 – Nunziata Giuseppe

POS34 – Pace Annalisa (UniSA)

POS35 – Panzetta Edoardo (UnivAQ)

POS36 – Pellegrino Michele (CNR)

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POS39 – Riva Laura (POLIMI)

POS40 – Sangalli Umberto (UniMI)

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POS42 – Sole Roberta (UniCAL)

POS43 – Spirio Laura (UniBO)

POS44 – Trevisan Letizia (UniTS)

POS45 – Yuan Wang (UniPD)

POS46 – Xi Menghzen (UniBO)

POS47 – Piacenza Pietro (UPO)

POS01

Sustainable materials for a greener future

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The growing demand for smart electronics, particularly wearable sensors embedded in textiles and garments, calls for innovative solutions that go beyond traditional rigid electronic platforms. Conventional materials and fabrication methods fail to meet the flexibility, sustainability, and seamless integration requirements of modern wearable devices. Moreover, the materials currently in use are neither sustainable nor recyclable, which also raises environmental concerns. This research is structured around three fundamental pillars aimed at advancing sustainable soft electronic platforms [1]. First, it addresses the reuse of plastic waste through the incorporation of bio-based chain extenders, such as mellophanic dianhydride [2], to recover and enhance the properties of discarded polymers. Second, it focuses on the development of flexible and reversible films by modifying protein-based matrices with functional groups capable of undergoing Diels–Alder reactions [3], enabling the formation of dynamic covalent networks. Third, it explores soft composites composed of rubber matrices and bio-derived fillers, also functionalized with Diels–Alder reactive moieties, to achieve reprocessable and adaptable materials. Together, these approaches aim to create a versatile platform combining recyclability, flexibility, and high performance for next-generation soft electronics.

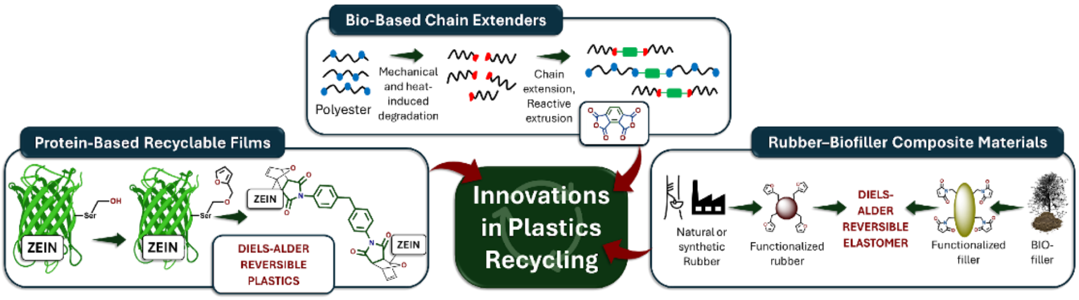

Figure 1. Sustainable materials strategies.

Financial support from: European Union's Horizon Europe research and innovation ECOTRON - grant agreement No 101070167, Circular Economy Lab for Life Sciences-CELLS within the MUSA–project–NextGenerationEU, PNRR, Mission 4 Component 2 Investment Line 1.5, PRIN 2022 PNRR "MadABio" CUP D53D23017110001, is gratefully acknowledged.

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POS02

Photochemical reactions: a powerful tool for the functionalisation of aromatic compounds

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The Friedel–Crafts reaction, one of the earliest examples of Lewis acid-promoted transformations, has long been a key method for forming C–C bonds. Traditionally, it requires a catalyst to proceed, including Lewis acids such as $AlCl_3$, $FeCl_3$, BF_3, $ZnCl_2$, and $TiCl_4$; Brønsted acids like HF, H_2SO_4, and H_3PO_4; as well as acidic oxide catalysts such as silica–alumina and cation-exchange resins. However, due to the harsh and often environmentally unfriendly conditions associated with these classical methods, alternative strategies have been actively explored. In this context, photocatalysis has emerged as a powerful and sustainable approach for C–C bond formation, enabling the generation of reactive radical intermediates under mild conditions using visible light.

In photocatalysis, there are many methods to generate carbon, oxygen, or nitrogen radicals. In recent years, the use of thianthrenium salts[1] has emerged as a powerful method to obtain these compounds. This work focuses on the development of a metal-free alkylation method for aromatic rings through the formation of electron donor–acceptor (EDA) complexes[2], using photochemical activation and carboxylates. Thianthrenium salts are employed to establish tight ion-pair interactions with carboxylates, leading to the formation of the desired products. In the Figure 1 the general reaction scheme is summarized.

The approach enables efficient alkylation even in the presence of electron-withdrawing groups, which typically reduce the reactivity of the aromatic ring toward electrophilic substitution. Various sulfur-based compounds, such as thianthrene, dibenzothiophene, phenoxathiine, and tetrafluorothianthrene, are explored for this purpose.

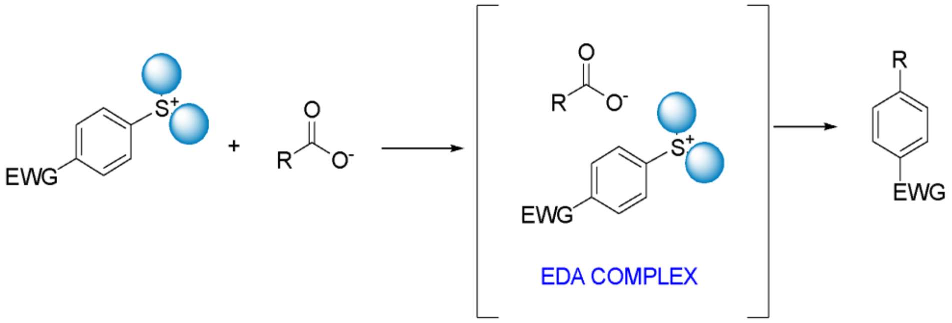

Figure 1: General reaction scheme for the reaction under study

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POS03

Development of rhenium-tricarbonyl complexes as potential IR bioimaging probes

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Diagnostic agents are essential tools in both biomedical research and clinical applications, enabling the visualization and detection of biomolecules within cells and tissues. Among them, metal-carbonyl complexes have emerged as promising candidates for bioimaging due to their unique chemical properties, including stability and the ability to be functionalized with biologically relevant moieties. These complexes, which feature transition metal centers (such as rhenium) coordinated with carbonyl (CO) ligands, exhibit strong absorption bands in the infrared (IR) spectrum, particularly in the 1900–2100 cm^{-1} region [1]. This spectral range lies within the cellular IR transparency window (1800-2200 cm^{-1}), enabling non-invasive imaging of biological tissues, which exhibit minimal absorption in this region. This study focuses on the development of novel molecular probes based on rhenium-tricarbonyl complexes designed to absorb within this IR window. A key aspect of our research is the application of a three-component reaction to synthesize cyclopentadienyl rhenium tricarbonyl ($CpRe(CO)_3$) derivatives [2]. This one-pot synthetic approach involves the reaction of a $Re(CO)_3^+$ precursor with a cyclopentadiene donor and a nucleophile, offering a rapid and efficient strategy to obtain functionalized metal complexes. Initially, we employed boronic acids as nucleophiles in the three-component reaction to synthesize glycoconjugated $CpRe(CO)_3$ derivatives. The obtained $CpRe(CO)_3$ complexes were subjected to preliminary biological assays, which revealed promising results in terms of their potential bioimaging applications. However, the use of boronic acids in the three-component reaction presented limitations, including instability of the precursors and synthetic challenges in their preparation. Building upon these findings, we explored terminal alkynes as stable and accessible carbon-based nucleophiles within the three-component reaction. Their direct use significantly streamlined the synthetic route for obtaining rhenium complexes, reducing the number of steps required and overall costs. This approach represents a potential new strategy for the development of innovative $CpRe(CO)_3$ probes that leverage IR spectroscopy for biomedical imaging applications.

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POS04

Synthesis and characterization of carbon-supported Vanadium species as new electrolytes for Vanadium Redox Flow Batteries

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Nowadays, our Earth is facing the problems coming out from Climate Change due to the enhancement of GHG emissions. Despite the necessity to decarbonize the industry production, developing new technologies based on renewable energy power generation sources, which are not constant and in some case unpredictable, requires high storage capacity. The most common way to store energy is using batteries, among them Flow Redox Batteries are in development as the most promising candidates for large-scale electrical energy storage systems requiring 6 or more hours of storage capacity, as is the case for most solar and wind energy storage applications. Vanadium Redox Flow Batteries (VRFB) have been undergoing development for the last 30 years, and have been found most appealing because both the anolyte and catholyte employ the same element, namely vanadium, which can exist in several oxidation states (V^{5+} to V^{2+}). However, the low energy density and the fact that vanadium is listed by Europe as critical raw material emphasize the need to enhance the sustainability and efficiency of VRFB technologies. The AIM of this work is to increase the concentration of the Vanadium redox centres beyond their solubility limits by adopting so called semi-solid electrolytes. These electrolytes are suspensions of carbon particles decorated by Vanadium-species. Our approach even enables to avoid the use of strong acidic environments. Here, we report about the synthesis of new Vanadium-based solid and semisolid electrodes to develop a new generation of VRFB. To achieve this goal we studied two different carbons as support for V^{2+}/V^{3+} and V^{4+}/V^{5+} redox couples. The former is a commercial reference material and the latter is a bio-char lab-made. On top of them, two different deposition techniques have been tested reaching different loadings of vanadium species, with the scope to obtain loadings mimicking those in the electrolytes of the current generation of VRFB (e.g., around 1.5 mol/L of vanadium in pure water). The materials synthesized have been characterized by SEM, BET, and XRD analysis. Before testing, their stability has been evaluated in electrolytes solutions to assess the leaching of vanadium species from the support, followed by XRD, and SEM on the spent material and MP-AES on the liquid-phase. The preliminary electrochemical characterization of the V-decorated carbons is reported. The synthesized materials showed some interesting results that with further studies could lead to the development of a new generation of Vanadium Redox Flow Batteries that are more environmental friendly, recyclable and less toxic.

POS05

Quantum-chemical study of the gas-phase reaction between myrcene and nitrate radicals

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Monoterpenes are a class of biogenic volatile organic compounds (BVOCs) mainly emitted by vegetation into the atmosphere. This family of terpenes, which plays an important role in the formation of secondary organic aerosols (SOA), is usually degraded by reactions with the major atmospheric oxidants: hydroxyl radicals (OH), ozone (O_3), and nitrate radicals (NO_3). Among monoterpenes, myrcene is one of the most abundantly emitted species. Previous studies have investigated the products of myrcene reactions with OH radicals and O_3, highlighting their importance in SOA formation [1,2]. However, its nighttime oxidation mechanism, driven by the reaction against NO_3, remains poorly investigated.

In this work, we present a detailed computational investigation of the gas-phase reaction mechanism between myrcene and the NO_3 radical. We started by carrying out a conformational analysis to identify and select the most stable conformers to consider for the reactivity study. For each conformer, NO_3 addition to the six available unsaturated carbon atoms was simulated, and the corresponding adducts and transition states have been identified. Structures of all stationary points found on the reactive potential energy surface (PES) have been optimized at both PW6B95/jun-cc-pVTZ and rev-DSD-PBEP86/jun-cc-pVTZ levels of theory, followed by harmonic frequency calculations. Both functionals have been augmented for dispersion interactions through the DFT-D3 scheme [3].

The different reaction channels and the corresponding thermochemical parameters are presented and discussed, along with subsequent reactive steps. In fact, the obtained PES represents the starting point in exploring the mechanisms leading to the formation of highly oxygenated organic molecules (HOM) and their eventual contribution to SOA production.

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POS06

Synthesis and antifungal activity of ferulic acid dimers and derivatives

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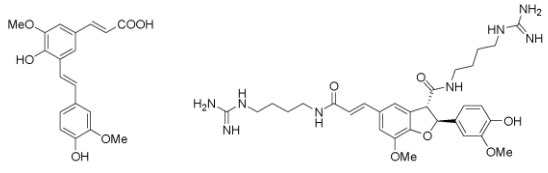
“Zero Hunger” represents a key priority among Sustainable Development Goals (SDGs) established by the UN Agenda 2030. Improving agricultural productivity and reducing food losses are indispensable; however, phytopathogens are still a major threat for food security. While synthetic pesticides remain the most effective tool for controlling crop diseases, their misuse has facilitated the emergence of multi-drug-resistant (MDR) microorganisms, highlighting the need for new, efficient and low-risk antimicrobials. Plant specialized metabolites involved in growth and plant-defense, known as phytoalexins and phytoanticipins, represent a valuable source of bioactive compounds. An excellent example are ferulic acid dimers, identified in the cell walls of barley and other grasses, which have shown antifungal potential [1]. In particular, poacic acid is believed to interfere with chitin production and β-1,3-glucan synthesis in fungal cell wall and with metal homeostasis [2].

In this context, a collection of ferulic acid dimers and derivatives have been synthesized and their antifungal activity has been evaluated *in vitro* against mycelium growth of some phytopathogenic fungi (*Botrytis cinerea*, *Pyricularia oryzae* and *Fusarium culmorum*) and on *P. oryzae* spore germination and appressorium formation. Overall, significant antifungal activity was observed for most of the assayed compounds. Appressorium formation, a specialized structure responsible for the fungal virulence, is promoted by an iron-mediated programmed cell death of conidia (ferroptosis). Considering that, the synthesis of iron-chelating compounds was identified as a sound strategy for the development of antifungal agents [3]. Hybrid metal chelators were then designed by combining poacic acid with nature-inspired siderophores aiming at obtaining multiple-target molecules to minimize the resistance emergence in phytopathogenic agents.



poacic acid **hordatine C**

Figure 1: Examples of natural ferulic acid dimers

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POS07

Toward the stereoselective synthesis of *ascaulitoxin aglycone*: a phytotoxin for sustainable weed control

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Weeds represent a major agricultural and environmental challenge, typically controlled with agrochemicals that pose risks to human and animal health. As an alternative, phytotoxins produced by plant pathogens offer environmentally friendly and highly specific solutions for weed management. Among these, ascaulitoxin and its aglycone (AscA)—potent bis-amino acid phytotoxins from *Ascochyta caulina*—have emerged as promising candidates for biocontrol of weeds[1,2]. However, the absolute and relative configurations of this unusual amino acid remain uncertain[3]. Developing an efficient synthetic route to all stereoisomers would enable configuration assignment, support structure–activity relationship studies, and provide sufficient quantities for large-scale applications. Here, we describe an initial approach to the diastereo- and enantioselective synthesis of ascaulitoxin aglycone (Figure 1). *Threo* isomers were accessed via asymmetric dihydroxylation followed by Mitsunobu azidation, whereas *erythro* isomers were obtained through direct asymmetric aminohydroxylation, both starting from the same olefin readily derived from Boc-L-allylglycine by esterification and cross metathesis.

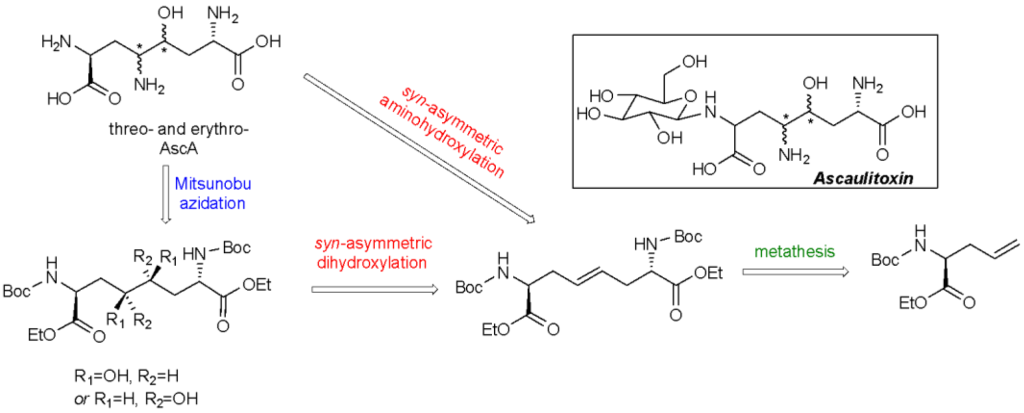

Figure 1: Structure of ascaulitoxin and its aglycone and retrosynthetic analysis

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POS08

Rapid access to bridged tricyclic systems involving an intramolecular Diels-Alder domino reaction as key step

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The creation of novel and structurally diverse molecular architectures with significant steric demand is of growing interest in modern organic chemistry, particularly due to their potential applications in the development of new materials and drug discovery. In this context, the combination of domino processes, a versatile strategy for constructing polycyclic systems with high atom- and step-economy [1], and electrochemical approaches, an efficient and sustainable method to access complex molecules without the need for stoichiometric amounts of hazardous oxidants or reductants [2], represents a promising pathway to achieve these goals. Among the various types of reactions employed in domino sequences, Diels–Alder cycloadditions have found widespread application in the construction of cyclohexenyl frameworks, which serve as key intermediates in the synthesis of certain classes of natural products [3].

The reaction of *N*-allyl-2-aminophenols and *O*-allyl-catechols under galvanostatic conditions in the presence of a nucleophilic species led to a domino sequence involving electrooxidation/nucleophilic addition/intramolecular Diels–Alder (IMDA) cyclization, affording compounds **1**. In the absence of a nucleophile, the reaction proceeded through an electrooxidation/IMDA sequence to yield compounds **2**, which are unfunctionalized at the α-position to the carbonyl group (Figure 1).

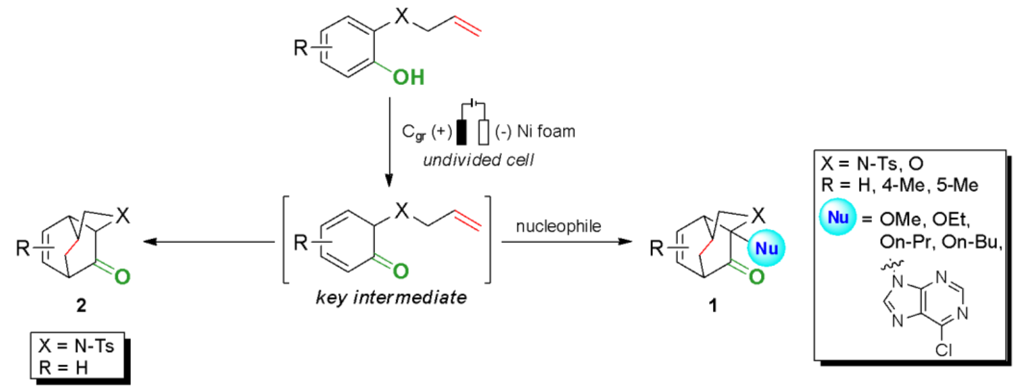

Figure 1: Scope of the domino process under electrochemical conditions on *N*-allyl-2-aminophenols and *O*-allyl-catechols.

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POS09

Silicon-carbenoid-mediated chemoselective and regiospecific homologative arylation of (benzo)pyridines

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The direct insertion of a CH_2X unit into an existing linkage enables the formal introduction of the targeted moiety with the predefined degree of functionalization [1]. Upon the fine tuning of the reaction conditions, the initial homologation event can serve as the manifold for triggering unusual rearrangement sequences leading to complex architectures through a unique synthetic operation [2].

Herein, we report the finely controlled installation of a functionalized methylene unit at the C2 position of (benzo)pyridine *N*-oxides with a novel versatile class of silicon carbenoids. The transformation, which occurs through a cascade of events involving homologation, intramolecular halogen displacement and deoxygenation/re-aromatization of the heterocyclic ring, provides highly functionalized 2-(aryl)methyl derivatives under full chemocontrol.

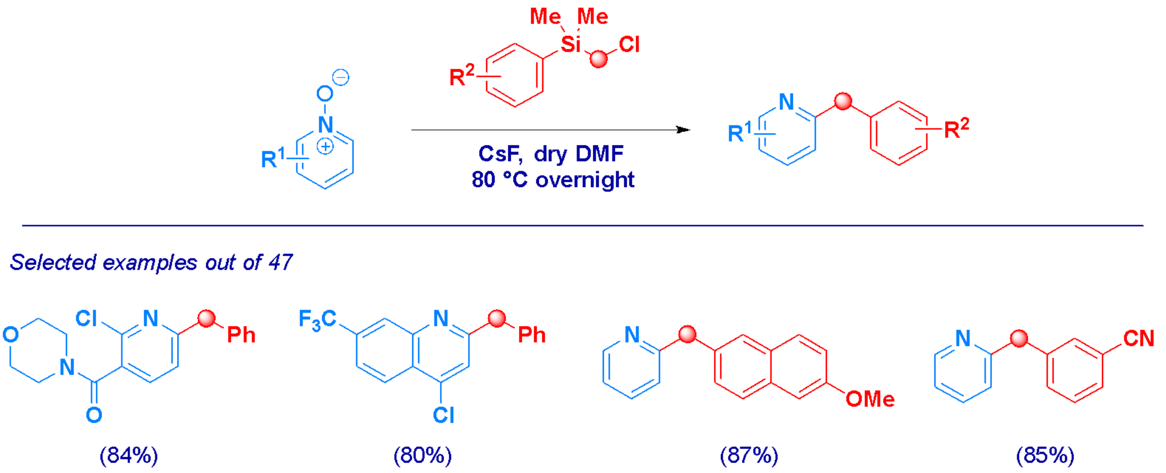

Figure 1: Silicon-carbenoid-mediated homologative arylation of (benzo)pyridines.

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POS10

Design rules for Maltodextrin-based electrolyte for aqueous Dye-sensitized Solar Cells

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As demand grows for autonomous low-power electronics—such as sensors, wearables, and IoT devices, indoor photovoltaics (IPV) are becoming a key enabling technology. Among the various IPV technologies, Dye-Sensitized Solar Cells (DSSCs) have shown significant promise due to their high efficiency under ambient lighting, low fabrication cost, and mechanical flexibility.[1] However, state-of-the-art DSSCs electrolytes typically rely on redox mediators dissolved in volatile and toxic organic solvents. These pose safety and health risks in enclosed indoor environments and contribute to limited long-term stability due to solvent evaporation and leakage.[2] To address these challenges, bio-derived *quasi*-solid-state electrolytes—particularly those based on polysaccharides—offer a sustainable and safer alternative. While outdoor and indoor PCEs of 7–8% and up to 20%, respectively, have been reported using such materials with thermal stability up to 60 °C and operational lifetimes >1500 h,[3,4] most systems rely on unmodified polysaccharides and lack a systematic study for optimization.

In this study, we present a rational design approach for aqueous *quasi*-solid electrolytes using maltodextrin-derived nanosponges with tailored cross-linking densities. These were structurally characterized (*e.g.,* TGA, FTIR-ATR, BET) and used to formulate gel electrolytes with water as a solvent (the safest in indoor conditions) and an iodine-based redox couple, chosen for its established reference behavior. The electrolytes were subjected to comprehensive electrochemical characterization, including electrochemical impedance spectroscopy (EIS), Tafel polarization, and ionic conductivity measurements. These were integrated with full DSSCs device testing under outdoor and indoor illumination conditions, evaluating Voc, Jsc, fill factor, and overall power conversion efficiency (PCE). Notably, the optimized *quasi*-solid electrolytes achieved a >15% increase in PCE that is maintained also after 200+ hours. Self-stability upon thermal stress up to 60°C has been tested also.

Finally, a Principal Component Analysis (PCA) was employed to correlate structural and rheological properties (*e.g.,* swelling ratio, Tg, porosity, viscosity) with key electrochemical and photovoltaic metrics, enabling the identification of dominant factors controlling performance. This data-driven approach provides quantitative design guidelines for future electrolyte development, highlighting the tunability of polysaccharide-based matrices for indoor photovoltaic-specific operating conditions.

Overall, this work advances the field by combining biopolymer engineering, electrochemical analysis, and multivariate data modeling to deliver safe, stable, and high-performing electrolytes for indoor DSSCs.

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POS11

Influence of the pH on the structure of $Zn(OH)_2$ precipitates during sealing post-treatments of PEO coatings

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Sealing is a post-treatment, typically combined with a previous surface process such as anodizing or plasma electrolytic oxidation (PEO), which is employed to improve the corrosion resistance of the treated component. Anodized and PEO coatings [1] are generally characterized by a high degree of porosity. The presence of pores or other defects compromises the anticorrosion effect of the coatings, since aggressive species may penetrate through them. To mitigate this issue, coated components are subjected to post-processing by sealing. One of the simplest sealing treatments is immersion sealing, in which the coated

sample is immersed in a heated, typically water-based, solution. During immersion, hydrated products are formed and precipitate within the defects of the coating, thereby clogging them. As a result, the physical barrier effect of the coating is enhanced, and its protective behaviour is improved. By modifying the chemical composition of the sealing solution, different insoluble compounds can be produced that precipitate into the pores; for example, common types of sealing are based on rare-earth or zinc salts [2]. In addition to bath composition, the pH of the solution is a fundamental parameter influencing the formation of hydrated products. The present work analyzed the influence of pH on the chemical reactions leading to $Zn(OH)_2$ precipitation and on the structures of the final hydrated products. The sealing post-treatment was carried out on PEO-coated samples produced from the magnesium alloy AZ31. These specimens were immersed in a $Zn(NO_3)_2$ solution heated to 90–95 °C. The evolution of the pH during processing and the chemical reactions leading to $Zn(OH)_2$ precipitation were evaluated. Different solution pH values ranging from 7 to 11 were tested. It was found that at low pH, the precipitation of hydrated species was hindered, whereas under alkaline conditions, $Zn(OH)_2$ lamellae were produced. The higher the pH, the more numerous and larger the lamellae.

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POS12

Expanding epigenetic modulation through LSD1 PROTACs

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Targeted Protein Degradation (TPD) is a cutting-edge strategy that selectively eliminates disease-causing proteins via the ubiquitin-proteasome system. PROTACs (PROteolysis TArgeting Chimeras) represent a leading approach within this emerging field. These hetero-bifunctional molecules simultaneously bind a protein of interest and an E3 ligase, inducing ubiquitination and subsequent proteasomal degradation of the target [1].

This work focuses on the development of novel PROTACs targeting lysine-specific demethylase 1A (LSD1), a FAD-dependent epigenetic enzyme involved in gene regulation and linked to cancer progression [2]. We developed two PROTAC series by selecting an irreversible and a reversible LSD1 ligand to investigate covalent and non-covalent binding modalities, respectively. Each series comprises analogues recruiting either the Cereblon or VHL E3 ligases, via pomalidomide or VHL-L1 ligands. Degradation and cell viability assays were performed in acute myeloid leukemia and medulloblastoma cells to evaluate the compounds' effects on LSD1 levels and cellular response.

The results highlight LSD1-targeting PROTACs as a promising avenue for further development in anticancer drug discovery.

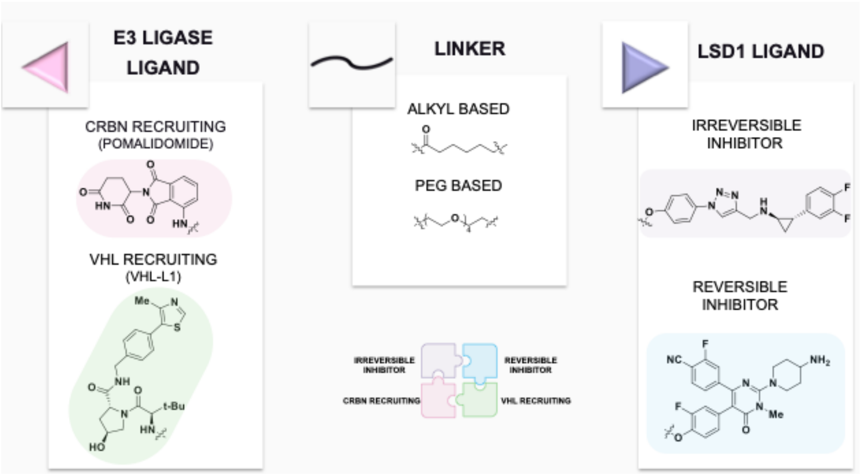

Figure 1 : Design strategy of potential LSD1-targeting PROTACs

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POS13

Hydrogen concentration Profile Prediction in Pipeline Steels: A Finite Element Modelling Approach Based on Experimental Diffusion Coefficients

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The accurate determination of hydrogen diffusion coefficients in pipeline steels is essential for predicting hydrogen distribution and assessing material performance in hydrogen-rich environments. This study focuses on measuring the hydrogen diffusion coefficient in commonly used pipeline steels (such as API 5 CT T95, P110 and API 5L X60) through electrochemical permeation tests performed according the Devanathan-Stachurski technique [1]. To extend the understanding of hydrogen diffusion beyond experimental measurements, Finite Element Modelling (FEM) was employed to study hydrogen concentration profiles within steel samples under various charging scenarios. The FEM simulations incorporated the experimentally derived diffusion coefficients, allowing for accurate prediction of hydrogen distribution profiles as a function of time and environmental conditions [2]. The combined experimental and numerical approach enables optimization of pre-charging conditions and helps in the evaluation of hydrogen embrittlement risks by providing detailed insights to improve material selection, design, and integrity management strategies for pipelines operating in hydrogen-containing service environments.

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POS14

Bioactive glass nanoparticles: from batch synthesis to an in-flow approach

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Silica bioactive glass nanoparticles (BG NPs) represent the latest advancements in sol-gel derived nanomaterials, offering large surface areas and porosity. These materials can be doped with a wide range of biologically active ions, enhancing their potential in soft and hard tissue repair and engineering [1,2]. Microfluidics has emerged as a promising tool for the in-flow production of NPs, offering greater control and reproducibility over conventional methods [3]. This work aims to design BG NPs, through the optimization of in-batch and in-flow processes. In the batch approach, four formulations of BG NPs, all containing SiO_2 and CaO, were synthesized through a sol-gel method *via* hydrothermal route and doped with different bioactive ions (P, Sr, or Zn) to investigate *in vitro* bioactivity, cytocompatibility, and antimicrobial properties. Meanwhile, in the in-flow approach, a PDMS-based microfluidic chip, conceived as sol-gel reaction device, was employed for the in-flow synthesis of SiO_2 NPs. The resulting BG NPs were characterized by TEM, SEM, and DLS. Moreover, to translate the batch synthesis into an in-flow approach, this process is currently being optimized by integrating the sol-gel microfluidic approach with the incorporation of biologically active ions such as Ca and Zn, facilitating the design of nanomaterials with tailored functions, ultimately improving NP performance in a variety of clinical applications.

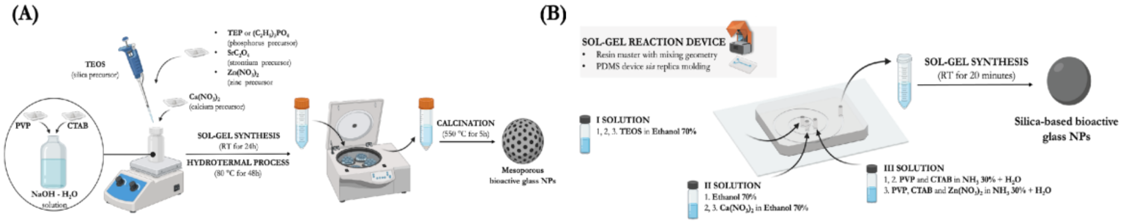

Figure 1: Experimental set up for the batch (A) and in-flow (B) synthesis of BG NPs.

This work was funded by the European Union - Next Generation EU, Italian NRP M4C2 Investment 1.5 “Rome Technopole: Innovation Ecosystem”, Project ECS 0000024 - CUP: C83C22000510001.

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POS15

Controlled aggregation of pyrene-based supramolecular nanostructures for light-driven switchable H_2 or H_2O_2 production

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Self-assembled organic chromophores form nanostructures in solutions, with their molecular packing determining the optoelectronic properties and photocatalytic activity [1,2]. In this work, we report an organic dye molecule, 1,3,6,8-tetrakis(4-ethynylbenzoic acid)pyrene (TEBAPy), that exhibits two aggregate states in aqueous conditions: nanofibers (NFs) and nanoparticles (NPs), depending on the charge-screening conditions (Fig. 1a) [3].

Interestingly, these two nanostructures were observed to be selective towards different photocatalytic products: the NFs promote sacrificial photocatalytic hydrogen production (H_2, 84 mmol g^{-1} h^{-1}) while the NPs produce hydrogen peroxide (H_2O_2, 71 mmol g^{-1} h^{-1}).

Interested in understanding the link between the morphology and the photocatalytic activity, we performed a combined spectroscopic and theoretical study. The aggregation-dependent photophysical properties were rationalized (Fig. 1b) as follows: the tightly packed morphology found in the NFs led to the strong mixing of the Frenkel and charge-transfer excitations (FE and CT, respectively), therefore favouring H_2 production, whereas the loosely packed structure of the NPs led to the formation of excitonic states localized within excited dimers, which were instead active for H_2O_2 production.

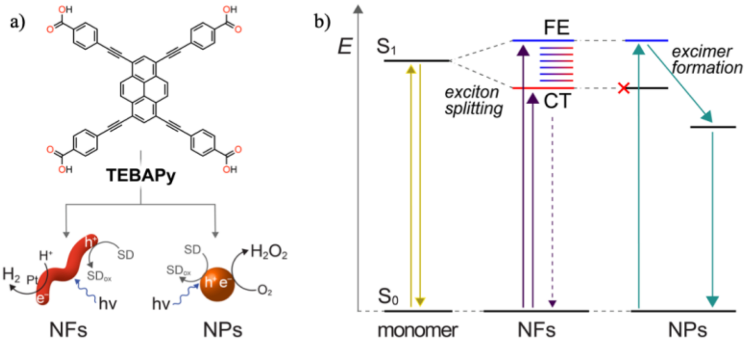

Figure 1: a) Schematic representation of TEBAPy's aggregates, which were exploited in this work as artificial photosystems for hydrogen (left) and hydrogen peroxide (right) production. b) Schematic representation of TEBAPy's aggregates excited state's dynamics.

[1] D. Cappelletti, M. Barbieri, A. Aliprandi, M. Maggini, L. Đorđević, *Nanoscale* 16 (2024), 9153-9168.
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POS16

Screening of small molecules libraries for the identification of novel pre-miR-21 ligands

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Dysregulation of miRNAs has been demonstrated to be a major factor in the development of some diseases, such as cancer, with miRNAs being recognized as oncogenic as their overexpression has been directly linked to cancer development. In this context, miR-21 is reportedly overexpressed in glioblastoma cells making it and its precursor, pre-miR-21, a potential therapeutical target[1].

Aiming to identify alternative compounds capable of inhibiting oncogenic miR-21 biogenesis, we carried out a screening of small molecules libraries for the binding with pre-miR-21 and the capability to interfere with Dicer-mediated cleavage.

Binding potential was evaluated through a Fluorescence Indicator Displacement (FID) assay: the identification relies on a change in fluorescence upon binding by displacing a non-selective RNA-binding dye, TO-PRO-1 (Figure 1a).

Inhibition of the Dicer enzyme cleavage was identified through a fluorescence resonance energy transfer (FRET)-based assay using a pre-miR-21 molecular beacon, labelled with a fluorophore (fluorescein or FAM) and a quencher (dabcyl or DAB). In the presence of recombinant Dicer enzyme, the RNA is cleaved, and an increase of fluorescence is detected. If the ligand is able to strongly bind the pre-miR-21 beacon, no fluorescence is detected (Figure 1b)[2]. The identification of small molecule pre-miR-21 ligands able to inhibit Dicer cleavage can pave the way to the development of novel potential chemotherapeutic treatment of glioblastoma.

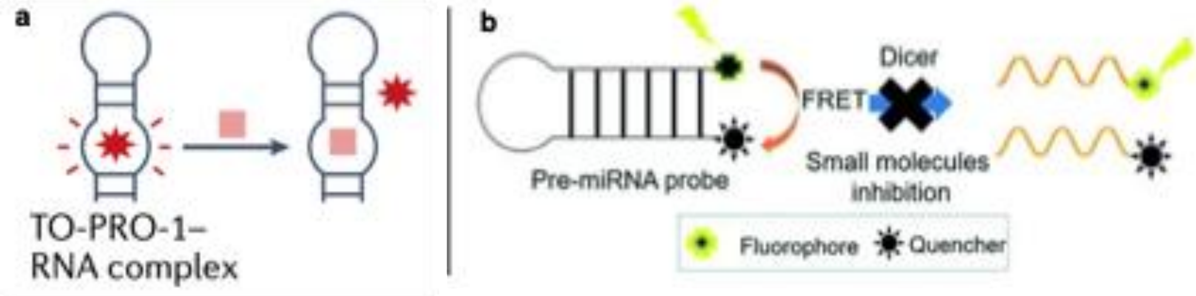

Figure 1: a) FID assay: increase of fluorescence is detected upon displacement of TO-PRO-1 by the binding of the ligand to the RNA target. b) FRET-based assay: increase of fluorescence is detected of Dicer enzyme is not inhibited.

Acknowledgments: This work was supported by "Fondo di Beneficenza Intesa San Paolo" (project no. B/2024/0249).

POS17

Sustainable conversion of anthocyanins into pyranoanthocyanins for textile applications

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[b] CNR-IPCB, Via P.Gaifami 18, 95126-Catania, Italy
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The textile industry has a significant environmental impact, particularly during the dyeing and finishing stages, where detergents, water repellents, and synthetic dyes often contaminate wastewater [1]. Nowadays, there is an increasing interest in sustainable, natural dyeing alternatives. Anthocyanins, a group of phenolic compounds, have emerged as a promising option [2]. To support a circular economy, compounds from food waste, such as grape pomace, are extracted using Natural Deep Eutectic Solvents (NADES). Whit their low toxicity, NADES can be combined with ultrasound to enable a more sustainable extraction method. Different acidic NADES were tested to find which gives the highest extraction yield. Since anthocyanins are unstable outside their natural environment, especially when exposed to light and heat, the goal of this project is to change them into pyranoanthocyanins, which are more stable and have stronger colours. Pyranoanthocyanins result from the attack of an enol form of a carbonyl compound or a vinyl group on the electrophilic C-position of the anthocyanin flavylium ring [3]. This study reports the synthesis of different pyranoanthocyanins and their characterization by LC-MS analysis.

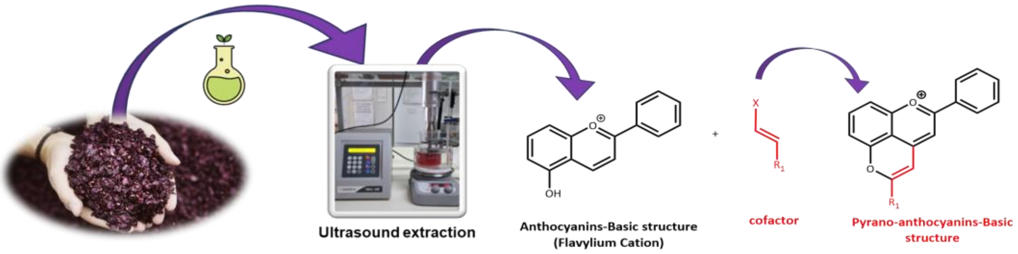

Figure 1: Scheme of anthocyanins extraction and chemical modification.

Letizia Fusto is thankful for the PhD grant (D.M. n 630, 24/04/24 Missione 4 “Istruzione e Ricerca” Componente 2– Dalla Ricerca all’Impresa, Investimento 3.3; PhD in Chemical Sciences, XL Cycle) financed by the Italian Ministry of University and Research (MUR). This work was financed by MUR ITALY PRIN 2022 PNRR (P2022MWY3P) macrosector “PE - Physical Sciences and Engineering.” Entitled: “Old but Gold! Identification of molecular platforms for age-associated diseases to promote healthy and active aging.” D.D. 1409 of 14/09/2022 - PNRR for Mission 4, Component 2, Investment 1.1.

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POS18

3,5-Dimethylpyrrole derivatives as potential dual modulators of mPGES-1 and sEH

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The simultaneous inhibition of microsomal prostaglandin E synthase-1 (mPGES-1) and soluble epoxide hydrolase (sEH) represents an emerging strategy for the development of novel anti-inflammatory and anticancer agents, as both enzymes play key roles in the regulation of lipid mediators involved in inflammation and tumor progression. A synergistic modulation of these two targets could enhance therapeutic efficacy while reducing adverse effects [1][2].

In a previous study [3], a series of pyrrole-based compounds was identified as dual inhibitors of mPGES-1 and sEH, exhibiting low micromolar IC_{50} values and validating this dual-targeting approach.

Building on these encouraging results, a new rational design project was undertaken to develop a library of substituted 3,5-dimethylpyrrole derivatives, featuring diverse amides at position 4 and aromatic ester-type substituents at position 2.

The study was conducted through a molecular docking-based virtual screening campaign; the items featuring the most promising docking score were further filtered after the visual inspection of the related poses, considering the key interactions with the macromolecular counterparts.

Preliminary modeling data revealed favorable binding orientations and interaction profiles consistent with dual inhibitory potential, supporting the interest in these new scaffolds as candidates for the development of multitarget agents.

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POS19

Tracking trace elements in biofouled plastics: a LA-ICP-MS approach

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Plastics in aquatic environments undergo aging processes that alter their physicochemical properties and interactions with the surrounding environment. Under biotic conditions, plastic surfaces were subject to microbial colonization, enhancing the adsorption, mobility, and release of trace elements, thereby affecting their environmental bioavailability [1]. Our experiments revealed that biofouled plastics exhibited higher adsorption rates of certain trace elements (e.g., copper (Cu)) compared to pristine, unaged materials. This result was obtained by quantifying the depletion of Cu in solution, as no conventional analytical techniques (e.g., ICP-MS) can differentiate between biofilm and plastics.

To shed light on the effect of biofilm on trace metal adsorption, a novel analytical approach—Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS)—was developed using artificially aged materials. Briefly, the analysis involves a depth profile analysis providing a vertical distribution of trace elements over a micrometric surface enabling to distinguish between the biofilm layer and bulk plastic. Polyethylene terephthalate (PET), polylactic acid (PLA) and polypropylene (PP) were selected in view of the presence of metal additives that can act as bulk plastic markers. Antimony (Sb) and tin (Sn) are abundantly present in PET and PLA, respectively, due to their use as polycondensation catalysts, whereas no specific markers are available for PP. Instead, Cu was selected as an indicator of biofilm presence due to its proven affinity for microbial colonies. The depth-resolved elemental profiling of both pristine and aged samples, allowed to clearly describe the role of biofilm in the adsorption process: the concentration of the biofilm marker decreases whereas those of Sb and Sn increases in function of the sampling depth. Such an evidence is practically blind by conventional analysis owing to the incapability to consider biofilm and plastics separately and to the extremely low amount of adsorbed species.

These findings highlight the critical role of biofilms in the interaction with trace metals, altering their environmental bioavailability. Furthermore, this study validates LA-ICP-MS as an effective technique for assessing in an accurate way the interactions between plastics and trace elements in environmental contexts.

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POS20

Harnessing acidic deep eutectic solvents for sustainable benzofuran synthesis

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Deep eutectic solvents (DESs) have emerged as promising green sustainable media, due to their low toxicity, biodegradability, ease of preparation, and multifunctionality, being able to act as both solvents and catalysts [1].

Benzofurans are widely important scaffolds in natural products, pharmaceuticals, and materials, with different biological activities, from antimicrobial to anticancer effects. Traditionally benzofurans are synthetized via base- or metal-promoted cyclizations of *o*-alkynylphenols and *o*-alkynylanisoles, but these approaches often rely on hazardous reagents or transition-metal catalysts [2].

In line with the pursuit of greener methodologies, our group has explored acidic DESs as active and recyclable media, often combined with microwave irradiation, for sustainable heterocycle synthesis [3]. A serendipitous observation during alkyne hydration revealed benzofuran formation from *o*-alkynylanisoles in acidic DESs. Building on this finding, we developed a selective and sustainable strategy for benzofuran synthesis in DES, representing the first example of their application to this transformation.

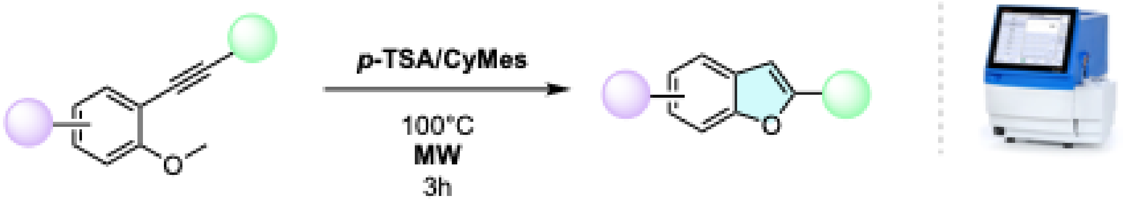

Figure 1: DESs-based MW-enhanced benzofuran synthesis

Herein, we are pleased to present the result of our investigation on the MW-enhanced DES-promoted cyclization *o*-alkynylanisoles to obtain substituted benzofurans (Figure 1).

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POS21

Transforming e-waste into value: ceramic capacitors as recyclable catalysts for the reduction of nitroarenes under mild condition

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This study explores the potential of electronic waste components as catalysts, with a particular focus on ceramic capacitors, key elements in motherboard circuits. Particularly, commercial ceramic capacitors (**CC**) and those recovered from waste motherboards, provided by a WEEE collection facility (**WC**), were studied. After grinding, the samples were characterized to identify the present metals using Scanning Electron Microscopy – Energy Dispersive X-ray Spectroscopy (SEM–EDX), Inductively Coupled Plasma – Optical Emission Spectroscopy (ICP–OES), and X-ray Diffraction (XRD). Based on thermogravimetric analysis (TGA), the optimal temperature was selected for calcination, allowing for maximum removal of plastic polymers from the sample. The magnetic fractions of calcined **CC** and **WC**, designated **MCC** and **MWC** respectively, proved active in the aqueous-phase reduction of nitroarenes to anilines at room temperature using sodium borohydride ($NaBH_4$) as a reducing agent. **MCC** retained catalytic activity over five cycles, and **MWC** over three. Control experiments confirmed the heterogeneous nature of the catalytic system, identifying copper (Cu) as the principal active species, with potential contributions from iron (Fe) and nickel (Ni).

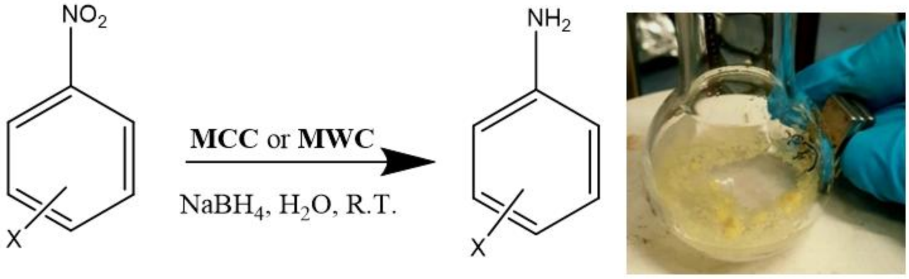

Figure 1: Reduction of nitroarenes catalysed by **MCC** and **MWC** and magnetic separation of the catalyst from reaction mixture

POS22

The role of quaternary amine functionalization in boosting the adsorption capacity of swellable organically modified silicas

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The widespread contamination of aquatic systems with toxic organic dyes, particularly azo dyes, such as methyl orange (MO), poses a significant environmental concern. Strategies for remediation that are based on adsorption, which make use of high efficiency and low-cost materials, offer a promising solution [1]. This study presents the synthesis and characterization of Quaternary Amino-functionalized Swellable Organically Modified Silicas (QA-SOMS) with different amounts of quaternary amine, prepared via a sol-gel process [2].

The physico-chemical properties of the materials were studied by using a multi-technique approach including elemental analysis, SEM, and N_2 physisorption to determine their composition, morphology, and textural properties. FT-IR, ss-NMR, and zeta potential analysis confirmed the successful incorporation of the quaternary amine groups and their impact on the surface charge, which is crucial for MO adsorption.

The adsorption performance of the materials toward MO was evaluated by using UV-Vis spectroscopy. A direct correlation between the increasing ratio of quaternary amine groups in QA-SOMS and the adsorption capacity was observed (Figure 1). The material with the highest functionalization achieved a remarkable capacity of 720 mg/g, highlighting QA-SOMS as a highly effective adsorbent for water remediation.

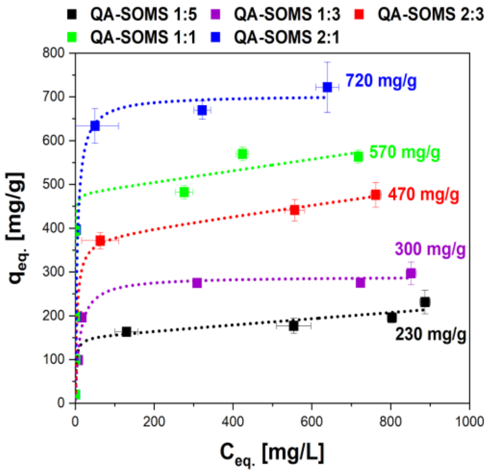

Figure 1: MO adsorption isotherms for QA-SOMS materials with varying quaternary amine amounts.

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POS23

Synthesis of putative ASIC3 channel activators against glioblastoma multiforme

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Glioblastoma multiforme (GBM) is the most common malignant primary brain cancer, characterized by high proliferation and infiltration, and remains incurable. Acid-Sensing Ion Channels (ASICs) are proton-gated cation channels expressed in various tumors and linked to increased cell migration and proliferation. Notably, the ASIC3 isoform, typically found in the peripheral nervous system (PNS) and absent in the central nervous system (CNS), is enriched in human GBM cancer stem cells (CSCs) but poorly expressed in the healthy human brain, making it a potential novel therapeutic target to control GBM CSC growth [1]. In vitro studies demonstrated that 2-guanidine-4-methylquinazoline (GMQ) significantly inhibited GBM CSCs growth, showing greater potency than the standard GBM drug, temozolomide (TMZ), and displaying a good safety profile on non-tumoral brain cells [2]. The present study focuses on the design and synthesis of novel GMQ-like scaffolds targeting glioblastoma, with enhanced blood-brain barrier (BBB) permeability. A key objective was the replacement of the highly basic guanidine moiety with a BBB-compliant guanylhydrazone surrogate (pKa 7-9), preserving bioactivity while improving CNS exposure. Furthermore, two focused libraries of substituted 2-methylquinazolines were synthesized, bearing the guanylhydrazone functionality either at the C-2 or C-4 position, depending on the adopted synthetic route (Figure 1). In vitro biological evaluation demonstrated significant anti-GBM growth for some analogues, reinforcing the therapeutic potential of this chemotype as a viable approach in the development of new treatments for glioblastoma.

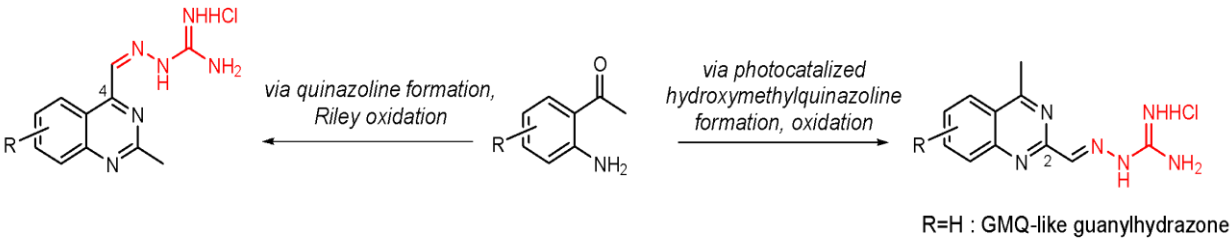

Figure 1: Representative structures of the synthesized 2-methylquinazoline derivatives bearing the guanylhydrazone moiety at either the C-2 or C-4 position.

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POS24

Ultrafast synthesis of tunable metal-decorated ZnO nanostructures for photocatalytic applications

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Hybrid semiconductor/metal nanostructures have attracted attention for their exceptional optical, electronic, and catalytic properties. Coupling semiconductor photocatalysts with plasmonic metals enhances charge separation and catalytic performance, yet challenges remain in synthesis, stability, and scalability.

Here, we present a rapid, sustainable, one-step method to synthesize piezoelectric zinc oxide (ZnO) nanostructures decorated with metal nanoparticles. Aqueous ZnO dispersions were treated with metal ions in an ultrasonic bath for one minute, enabling precise control of nanoparticle size and density through the metal ion concentration.

Preliminary studies with Au^{3+} confirmed successful Au decoration via spectroscopic and morphological analyses. The ZnO@Au hybrids were tested for H_2O_2 production and Cr(VI) photoreduction under solar-simulated irradiation, showing efficiency trends consistent with their structure and morphology.

Finally, we demonstrate the versatility of this approach using different metal precursors, underlining its potential for the design of a wide range of hybrid semiconductor materials.

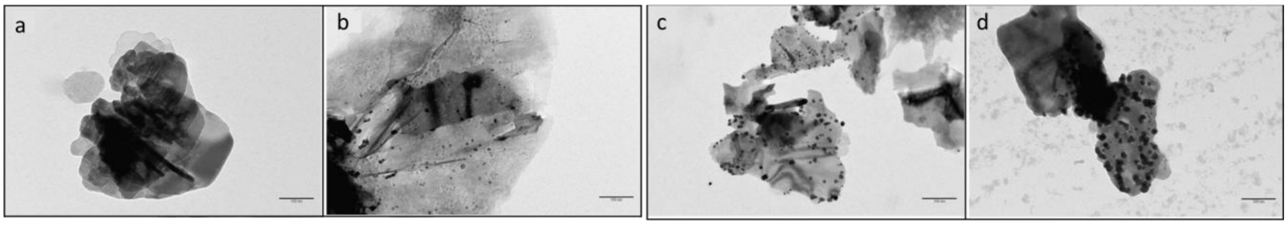

Figure 1: TEM images acquired for ZnO pristine (a)and ZnO with increasing concentration of Au nanoparticles (b-d).

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[2] R.H. Adnan and A.A. Jalil, *Mater. Today Chem.* 27 (2023) 101322.

POS25

Upcycling hop residues into antioxidant-enhanced biopolymer films for food packaging applications

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Modern agricultural technologies have boosted crop production but also caused lasting environmental, social, and economic impacts. Moreover, the 150 billion metric tons of agricultural waste generated annually are largely mismanaged through burning or landfilling, contributing significantly to pollution and resource inefficiency. However, these biomasses, dismissed as waste, contain valuable bioactive molecules with antioxidant, antimicrobial, and anti-inflammatory properties, offering great potential for chemical, cosmetic, and pharmaceutical applications.

Among the various agricultural residues, hop (*Humulus lupulus L.*) by-products such as branches, leaves, and cones discarded after harvesting, represent a rich yet underutilized source of bioactive compounds, specially flavonols, prenylflavonoids, and proanthocyanidins, known for their antioxidant, and antimicrobial activities [1].

These residues can be directly recovered and used as fillers in polymeric matrices, imparting intrinsic antioxidant functionality to the material. Hop byproducts (HBP) have been incorporated into a bioderived and biodegradable polymer, polybutylene succinate (PBS) to produce composite films in which HBP increased both the elastic modulus and water-absorption capacity. The antioxidant compounds within HBP remained active after incorporation and showed a favorable release behavior in food simulants. Due to their higher solubility in lipophilic environments, these films are particularly suitable as packaging for fatty foods, though their slower, controlled release also makes them effective for aqueous foods.

Harnessing hop residues not only reduces the environmental burdens associated with their disposal but also adds value to the brewing and agricultural industries through sustainable bioproduct development, while contributing to reduced food waste by limiting spoilage.

This work was carried out within the Agritech National Research Center (Task 8.1.3. Valorization of the waste to obtain biomaterials) and received funding from the European Union via Next-Generation EU (PIANO NAZIONALE DI RIPRESA E RESILIENZA (PNRR)—MISSIONE 4 COMPONENTE 2, INVESTIMENTO 1.4—D.D. 1032 17/06/2022022, CN00000022).

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POS26

Assessment of circularity requirements for rare earth permanent magnets in e-drive motors

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The electrification of the automotive sector has increased the EU's reliance on critical raw materials (CRMs) such as rare earth elements (REEs), Cu, Li, Co and Ni. This dependency underscores the need for a higher circularity in end-of-life vehicles. Building upon a previous report from the Joint Research Centre [1], this work elaborates on the measures proposed in the new End-of-Life Vehicle Regulation and aids its development by assessing new circularity measures for electric drive motors in vehicles [2]. The study also aligns with the CRM Act (CRMA) and the EU's strategic objectives. Here we developed a dynamic material flow analysis model to estimate the potential flows of e-drive motors and their permanent magnets (PMs) to be put on the market and available for collection and recycling, from 2010 to 2040 in the EU-27. We calculate the potential recycled content (RC) for the main REEs in PMs (i.e., Nd, Pr, Dy and Tb) in two forecast scenarios, based on different policy options, and investigate the technical feasibility of recycling efficiency (RE), material recovery level (MRL) and RC targets for these elements. The primary finding of the study is that the RC targets for REEs in passenger cars and vans are projected to reach, in 2040, a theoretical 15% in the least favourable policy scenario and 22% in the ideal scenario. These results are below the benchmark value for RC targets of 25% established in the CRMA, showing that prioritizing RE and/or MRL may be more effective in the short-medium term.

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POS27

First-principles Insights on Entropy-driven Mechanism in P2-Type Layered Oxides for Na-ion Battery Cathodes

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P2-type Na_xTMO_2 layered oxides ($x < 1$, TM = transition metal) are highly promising cathodes for Na-ion batteries due to their open Na^+ diffusion pathways and favorable electrochemical kinetics [1]. However, their practical deployment is hindered by phase transitions and TM migration during cycling, leading to capacity fading and voltage hysteresis [2]. Introducing configurational entropy offers a powerful route to enhance both structural stability and electrochemical performance, yet the mechanisms underlying these entropy-driven effects remain poorly understood [3].

By comparing three P2-Na_xTMO_2 materials with increasing compositional complexity, *i.e.*, $Na_{0.68}Mn_{0.68}Ni_{0.32}O_2$ (low-entropy oxide, LEO), $Na_{0.68}Mn_{0.44}Ni_{0.19}Co_{0.25}Ti_{0.09}Mg_{0.03}O_2$ (medium-entropy oxide, MEO), and $Na_{0.68}Mn_{0.44}Ni_{0.19}Co_{0.19}Ti_{0.09}Mg_{0.03}Al_{0.05}Fe_{0.01}O_2$ (high-entropy oxide, HEO), we elucidate the role of entropy in modulating the structural and electronic response upon charge. Higher configurational entropy is shown to delocalize the redox process across multiple electroactive species with charge compensation burden, thus leading to improved electrochemical stability, as revealed by hybrid-DFT calculations and CV profiles. Stable cycling and less favourable TM/Na_{vac} antisite defects formation suggest that TM migration and dissolution in the electrolyte can be effectively discouraged, enabling superior reversible capacity. When cycled with a room-temperature ionic-liquid (RTIL) based electrolyte, the high-entropy cathode features enhanced structural retention, confirmed by *ex situ* XRD, owing to the mitigated TM octahedral distortions and suppressed layer gliding dissected from first principles. These findings establish configurational entropy as a key design parameter for the development of durable, high-performance layered cathodes for next-generation Na-ion batteries.

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POS28

Gold-catalyzed cyclization reaction for the synthesis of biologically relevant polycyclic indole derivatives.

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The human immunodeficiency viruses (HIV) are two species of retroviruses responsible for AIDS. Despite the approval of several antiretroviral agents for clinical use, the efficacy of these treatments remains compromised because of drug-resistance and side effects associated with prolonged administration. As a result, there is still a high demand from both society and industry for the discovery and development of novel, selective, and safer compounds for HIV therapy [1]. In this context, 5,6-dihydroindolo[1,2-a]quinoxaline has emerged as a promising scaffold, demonstrating potent in-vitro antiretroviral activity against HIV-infected cells.

Considering these premises and the continuous interest of our research group in the synthesis and functionalization of complex indole derivatives, we have evaluated the possibility of constructing a new class of indolo[1,2-a]quinoxalines through the cyclization of N-(propa-1,2-dien-1-yl) derivatives under mild and safe catalytic conditions. This transformation exploits the well-established ability of gold to activate allenic bonds and has as main advantages high yields and selectivity. A library of targets with various structural modifications was synthetized, with the rationale in the promising pharmacological potential of this chemical framework, as antifungal and anti-retroviral agents. Moreover, our method showed high flexibility, as we could successfully apply it for the synthesis of 11H-indolo[3,2-c]quinolines, which is another important class of biollogically relevant indole derivatives.

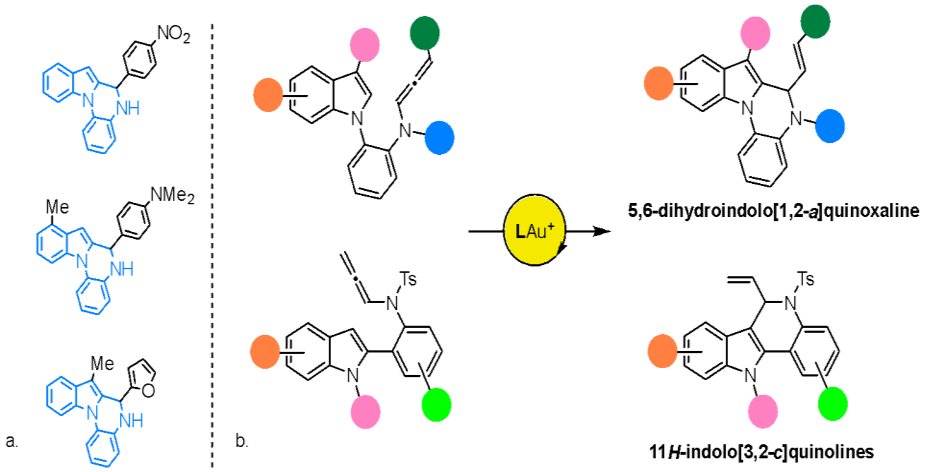

Figure 1: a. selected examples of 5,6-dihydroindolo[1,2-*a*]quinoxalines with *in-vitro* anti HIV activity; b. gold catalyzed synthesis of polycyclic indole derivatives.

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POS29

Rotational Motion in Bispidines: A Conformational Study

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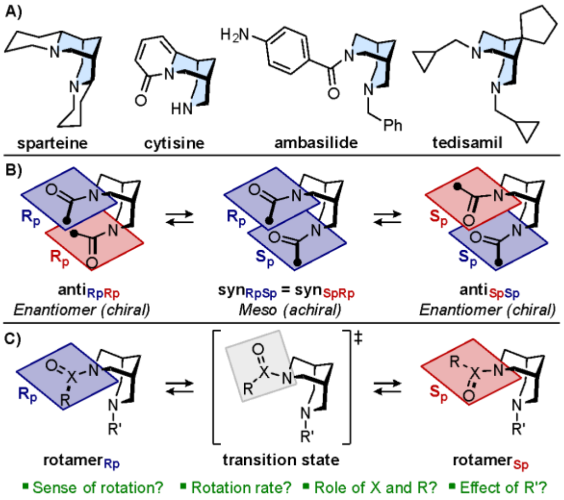
Bispidines are a class of bicyclic diamines characterized by two fused piperidine rings. Found predominantly in natural products, bispidines exhibit a range of pharmacological effects, making them of significant interest in drug design (Scheme 1A) [1]. Beyond their medicinal uses, bispidine structures have emerged as promising scaffolds in organocatalysis or molecular motors [2]. This is the case of bispidine diamides where the relative position of the two carbonyl groups is reminiscent of molecular machine with stops at the syn/anti position, thus allowing chiral–achiral switching (Scheme 1B) [3]. While various studies have investigated the relative positioning of the two amide groups, a detailed conformational analysis of rotameric bispidines beyond diamides has not yet been fully explored. In this work, a series of rotameric bispidines have been examined experimentally and computationally, revealing how intramolecular stabilizing effects play an essential role in determining observable rotational motion (Scheme 1C). Particular attention has been given to the factors influencing the rate and direction of rotation for different classes of bispidinic rotamers (*N*-Ac, *N*-Boc, *N*-NO). The conformational analysis was also supported by X-Ray Diffraction analysis and Variable Temperature NMR studies. The insights gained from this work aim to provide valuable guidance for the design of new molecular motors or organocatalysts, where the ability to control rotational movement is crucial to the function of the system.



Scheme 1. A) Examples of natural and synthetic relevant bispidines. B) Planar chirality in diacyl bispidine. C) Conformational study of rotameric bispidines (our work).

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POS30

From food waste to value-added compound: a circular approach

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The valorization of agri-food by-products is increasingly important in addressing global food demand, environmental sustainability [1], and circular economy goals [2]. This study discus valorization of orange by-products, which are typically discarded but represent valuable sources of polyphenols, flavonoids, dietary fibers, and pectins. Green extraction was carried out using ultrasound-assisted extraction (UAE), selected due to its efficiency, compound preservation, and reduced environmental impact. Response surface methodology was used to optimize the extraction method in order to maximize the total polyphenols content.

In parallel, pectin was extracted from orange by-products and both polyphenols and pectin were characterized by analytical techniques (LC-MS and FT-IR). Finally, Pectin Polyphenol Beads (PPBs) were obtained by ion gelation method and used as encapsulating agents for polyphenols, creating stable delivery systems to use in functional food or pollutant removal and stabilization processes. The dual strategy highlights a holistic valorization pathway for orange by-products, transforming waste into high-value compounds with food and environmental applications. The approach strengthens the link between circular economy principles, sustainability, and the One Health perspective.

Acknowledgment The research leading to these results has received funding from "ROBERTA-IntegRated apprOach to real eco sustainaBIE gReen TotAl index" CUP E53D23015670001, project number P2022HEBEX funded by EU in Next Generation EU plan through the ITALIA "PRIN 2022 PNRR" finanziato dall'Unione Europea.

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POS31

Development of Polyfunctional Heterocyclic Scaffolds as Inhibitors of pre-miR-21

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miR-21 is a well-established oncomiR that is frequently upregulated in solid tumors and neuroinflammatory conditions, where it promotes proliferation, invasion, and apoptosis resistance by targeting PTEN, PDCD4, and RECK [1]. Targeting the maturation of pre-miR-21 has emerged as a promising strategy to suppress its oncogenic functions in both peripheral tissues and the central nervous system. In 2008, Gumireddy et al. identified diazobenzene derivatives that inhibit Dicer-mediated processing of pre-miR-21 ($EC_{50} \approx 2$ µM) in luciferase and cell-based assays [2]. Subsequent work by Shi et al. introduced AC1MMYR2, which significantly reduces tumor growth and metastasis in orthotopic brain, breast, and gastric cancer models without notable systemic toxicity [3]. However, the high molecular weight and polarity of these inhibitors impede blood–brain barrier penetration. To address this, our group is developing piperazine-based small molecules designed for high-affinity pre-miR-21 binding coupled with optimized pharmacokinetic profiles for improved brain delivery.

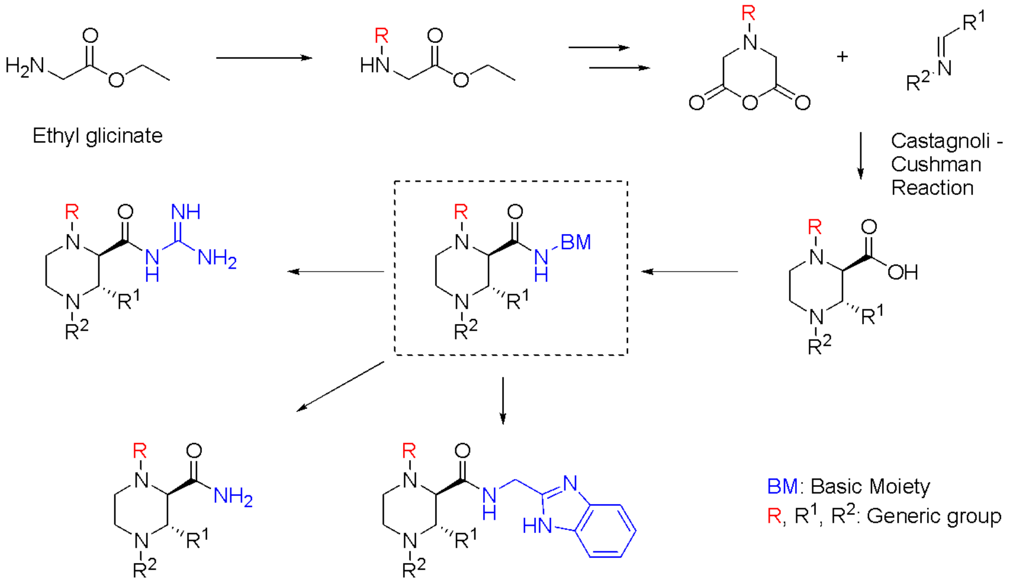

Figure 1: Synthetic strategy for diversely substituted piperazines.

Acknowledgments: This work was supported by "Fondo di Beneficenza Intesa San Paolo" (project no. B/2024/0249).

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POS32

Sequential ester homologation-nucleophile-guided functionalization: a chemoselective access to thioesters, amides, and acids

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Homologation chemistry represents a powerful approach for the stepwise extension of carbon frameworks, enabling the precise introduction of functionalized methylene units into diverse substrates. Particularly, the direct transfer of a nucleophilic CH$_2$X fragment into an existing molecular framework provides an efficient strategy for the formal introduction of this moiety with a precisely defined degree of functionalization [1]. By fine-tuning the reaction conditions governing this transformation, the initial homologation step can be exploited as a platform for triggering unconventional rearrangement pathways, thereby enabling the construction of structurally complex architectures through a single synthetic operation [2].

Herein, the homologation of esters to thioesters, amides, and carboxylic acid by mediated by lithium carbenoid is reported. By controlling the tetrahedral intermediate collapsing and promoting a series of rearrangements ultimately leading to a high electrophilic ketene, the subsequent incorporation of S-, N-, and O-nucleophilic elements furnishes the title compounds. Despite the coexistence of multiple (concomitant) equilibria and short living entities, the protocol features remarkable chemocontrol and flexibility. Notably, the formal oxidation state of the final compounds is retained.

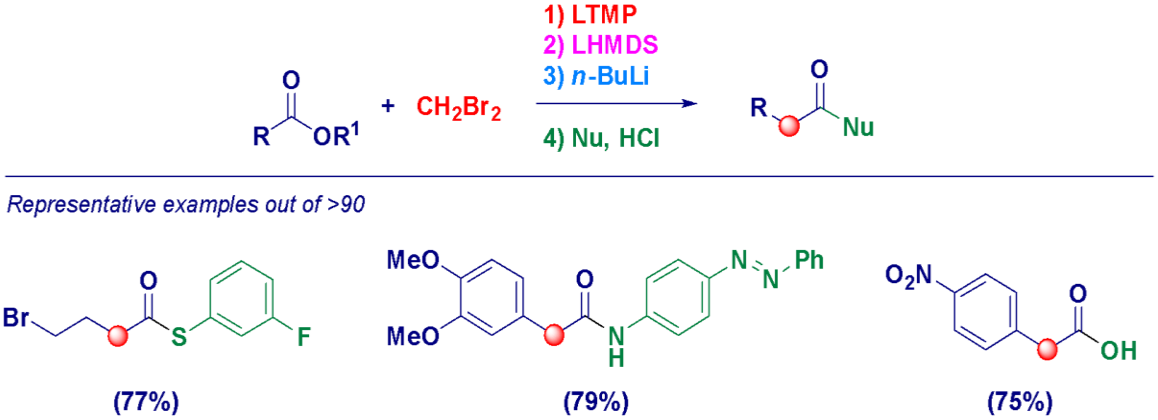

Figure 1: Esters Homologation to Carboxylic Derivatives.

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POS33

Design and Characterization of Jeffamine-based Nanogels for Biomedical Applications

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Nanogels represent a highly adaptable class of nanocarriers, combining the tunable physicochemical properties of nanoparticles with the structural flexibility of hydrogels. This unique hybrid architecture enables efficient drug encapsulation, protection against enzymatic degradation, and controlled release kinetics, making nanogels particularly attractive for drug delivery applications. Among the various formulations explored, polyethyleneimine (PEI)-based nanogels have been widely studied due to their strong cationic charge, which enhances nucleic acid complexation and cellular internalization. However, the high cytotoxicity and poor biodegradability of PEI significantly limit its clinical translation.

In this study, we report the design, synthesis, and comprehensive characterization of polyethylene glycol (PEG)-Jeffamine-based nanogels as a biocompatible and biodegradable alternative to conventional PEG-PEI systems. The synthetic strategy involved the epichlorohydrin-mediated activation of PEG, followed by azide functionalization and subsequent conjugation with Jeffamine via click chemistry. Jeffamine, a polyetheramine known for its favorable biocompatibility, was selected to minimize cytotoxicity while preserving functional versatility. Reaction success at each stage was confirmed via nuclear magnetic resonance (NMR) spectroscopy.

The nanogels were thoroughly characterized using dynamic light scattering (DLS), which confirmed narrow size distribution and high colloidal stability. Morphological analyses by transmission electron microscopy (TEM) and atomic force microscopy (AFM) revealed uniform, spherical nanostructures with well-defined surfaces. Drug encapsulation efficiency and release profiles were evaluated using Rhodamine B (hydrophilic) and Pyrene (hydrophobic) as model compounds. UV-Vis spectroscopy revealed enhanced encapsulation of Rhodamine B in PEG-Jeffamine nanogels compared to PEG-PEI systems, indicating superior affinity for hydrophilic drugs. Meanwhile, Pyrene exhibited a sustained release profile, consistent with its hydrophobic interactions within the gel matrix.

Biocompatibility was assessed using cytotoxicity assays on mammalian oligodendrocyte cultures. PEG-Jeffamine nanogels showed significantly reduced cytotoxicity relative to PEI-based controls, highlighting their potential for safe biomedical use. Overall, this study establishes PEG-Jeffamine nanogels as a promising platform for precision drug delivery. Their excellent biocompatibility, customizable release behavior, and extensive chemical flexibility position them as viable candidates for next-generation polymeric nanocarriers in applications ranging from oncology and gene therapy to regenerative medicine.

POS34

Synthesis, characterization, and photocatalytic performance of Nitrogen-doped Magnesium Oxide

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Metal oxides such as TiO_2, ZnO, MgO, and SnO_2 are characterized by properties such as high thermal stability, good reactivity, and biocompatibility, which make them suitable for applications in fields such as optics, sensing, electronics, and photocatalysis.

Among these, magnesium oxide exhibits a set of remarkable features, including wide global availability of raw materials, environmental compatibility, and non-toxicity, in addition to antimicrobial, antifungal, and antiviral properties that enable effective action against the proliferation of microorganisms [1]. These characteristics make magnesium oxide an excellent candidate for applications in the field of food packaging.

MgO is a wide band-gap semiconductor activated by UV light; therefore, under illumination limited to visible light, its effectiveness as a photocatalyst in degradation processes is almost negligible. With a view to its potential use in food packaging, and considering that packaged products in transparent containers are exposed only to visible light on store shelves, it is essential to expand the activation capacity of MgO's photocatalytic properties into the visible radiation range. This enhancement can be achieved by introducing metallic and/or non-metallic elements into the crystalline structure of the semiconductor, thereby reducing the band gap through the generation of energy levels between the valence and conduction bands [2].

The aim of this study was to optimize the photocatalytic properties of MgO under visible light through nitrogen doping, achieved using two different synthetic strategies. Specifically, one procedure was based on the thermal treatment of MgO precursors in the presence of gaseous nitrogen, while the other relied on the use of nitrogen-containing compounds as nitrogen precursors. The obtained samples were characterized structurally (via X-ray diffraction) and spectroscopically (via infrared and Raman analyses) in order to evaluate the effect of the two doping procedures on the physical properties of the materials. Finally, their ability to degrade a model organic pollutant, methylene blue, under visible light irradiation was compared.

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POS35

Computational study on N-methylacetamide (NMA) amide bond cleavage in alkaline medium

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The peptide bond is of crucial importance in the chemistry of proteins, since its nature regulates different biochemical processes. Although peptide bonds are very stable under physiological conditions, their cleavage can be accelerated by orders of magnitude by acting on temperature and pH. To date, few publications have been reported in the literature that have tried to explain the mechanism for the amide bond cleavage reaction [1]. In the present study, we apply a computational approach able to reconstruct the free energy profile of this reaction and the associated kinetic constants under alkaline conditions. That is, we apply the Perturbed Matrix Method (PMM), a theoretical-computational QM-MM approach that considers a system divided into two parts. Our work began with the study of a small model system with an amide bond to represent the peptide bond, N-methylacetamide (NMA), thus neglecting the presence of amino acids' lateral chains and conformational effects present in proteins. By means of PMM, we have modelled the entire mechanism of the reaction and estimated the reaction kinetics at 300 and 360 K, through Eyring and Landau equations. Our results are, within the statistical error, in reasonable agreement with data reported in the literature [2] and initial laboratory experiments.

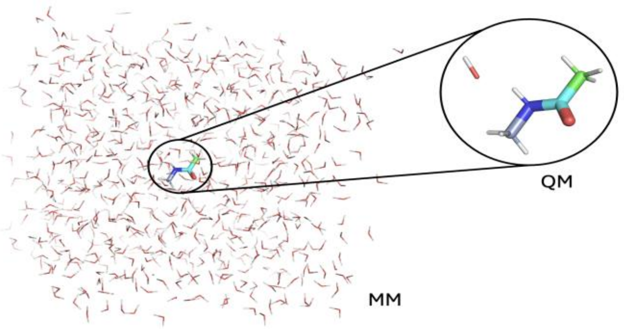

Figure 1: QM-MM scheme: quantum center represented by NMA and OH^-, environment by water molecules.

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POS36

LC-HRMS characterization of by-products of contaminants of emerging concern during TiO_2-based photocatalytic degradation in water

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One of the most long-standing problems related to climate change is the scarcity of water, which has a deleterious impact on various sectors, including agriculture, livestock, industry and public health. In this scenario, CECs removal processes have a huge potential for potable and non-potable reuse. The effectiveness of various photocatalytic systems for the degradation of a selected group of CECs (carbamazepine, diclofenac, irbesartan, sulfamethoxazole), particularly TiO_2 deposited on commercial humic acids (HA), has been evaluated. This treatment belongs to the Advanced Oxidation Processes (AOPs), whose purpose is to generate reactive oxygen species (ROSs) that can oxidize target compounds [1]. Photocatalytic systems TiO_2-based seem to be very promising considering their low toxicity, environmental friendliness and low cost, in addition to their high photocatalytic activity under UV/VIS irradiation. Downstream of these processes, attention should be paid to the transformation products (TPs) with unknown toxicity [2]. This study focuses on the characterization of the results of photocatalytic processes using high-resolution mass spectrometry (HRMS) coupled with liquid chromatography (LC). Reversed-phase liquid chromatography (RPLC) was employed with electrospray ionization (ESI)-HRMS. The approach named Suspect Screening (SS) was used for the identification of the degradation by-products arising from the selected CECs. Precursor compounds and associated by-products were identified by using mass spectrometry detection in positive-ion mode, during which the analytes were ionized as protonated adducts ($[M+H]^+$). TP structural elucidation was allowed by acquiring MS/MS spectra. Based on the accurate *m/z* values, the retention time matching with standard solution injection and MS/MS spectra, putative structures were assigned to some by-products [3], in particular oxidation products. Future perspectives include studying photocatalytic processes on real matrices and evaluating whether the matrix effect influences the degradation pathway of the CECs under study.

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POS37

Electrochemical decarboxylative C-N bond formation

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The carboxylic acids are featured with bench-stability, low cost, great structural diversity, non-toxicity and abundant commercial sources. Due to these remarkable properties, they are attractive synthetic feedstocks in the industrial landscape [1].

Recently, electrochemical approach has emerged as powerful tool in the decarboxylation reaction since it represents a mild and green strategy for the construction of new C-C and C-X (X= O, N) bonds obtaining CO_2 and H_2 as unique byproducts in the reaction [1].

The well-established Hofer-Moest reaction affords, after the double oxidation of the carboxylic acid, the formation of carbocation that could be intercept by a nucleophile to evolve in the desired product [3]. Based on this, our aim is to explore a novel electrochemical strategy starting from carboxylate anions to build C-N bonds.

To the best of our knowledge, effective electrochemical methodologies which employ acetonitrile or other nitriles as nitrogen source in this type of transformation are not reported yet. The reaction proceeds through the double oxidation mechanism where the carboxylate undergoes anodic oxidation to generate a radical followed by another oxidation to afford the carbocation which can be intercepted by a nitrile, and then, possibly, by a nucleophile to afford the new functionalized product.

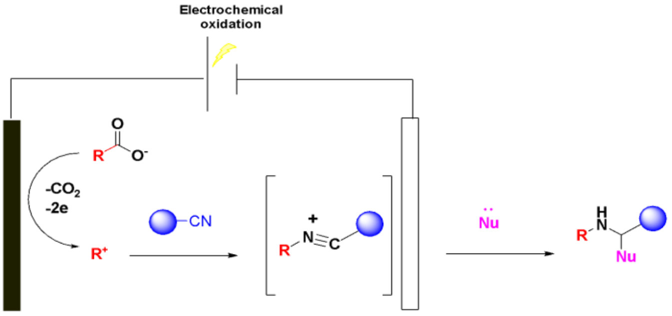

Figure 1: General reaction scheme for decarboxylative C-N bond formation.

Notably, in our studies in the presence of hexafluoropropanol, we observed the formation of unique and unreported intermediate when carboxylate substrates are treated with acetonitrile under electrochemical conditions. This intermediate can undergo further synthetic manipulations. These findings provide the bases towards a carboxylate-based amination strategies through electrochemical activation.

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POS38

Elemental composition and strontium isotope ratio determination in industrial hemp (*Cannabis sativa L.*) for textile applications

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This pilot study evaluates the feasibility of tracing the geographical origin of industrial hemp within the textile supply chain using isotopic and elemental determination. In particular, it focuses on the $^{87}Sr/^{86}Sr$ isotope ratio in combination with major, minor, and trace element concentrations in hemp samples collected from different Italian regions. An analytical protocol was developed and validated employing Multi-Collector Inductively Coupled Plasma Mass Spectrometry (MC-ICP/MS), Atomic Absorption Spectroscopy (AAS), and ICP-MS.

The results demonstrate that the $^{87}Sr/^{86}Sr$ isotopic ratio, integrated with elemental profiling, provides a robust tool for geographic discrimination [1]. Hemp from Northern Italy (e.g., Modena, Carpi, Parma [2]) exhibited consistent isotopic signatures, while samples from Southern regions showed distinct values, enabling clear regional differentiation. Elemental determination also highlighted variations along the plant stem and between different tissues.

Hazardous metals such as Hg, Pb, and Cd were detected at very low concentrations, confirming the environmental safety of the analyzed hemp [3]. Overall, the study demonstrates that isotopic and elemental indicators can effectively support the traceability and authenticity of textile hemp, contributing to a more sustainable and transparent supply chain in Italy.

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POS39

Green cellulose-based nanomaterials for the improved monitoring of water microbiological quality

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The SafeCREW EU project aims to support the implementation of the new EU Drinking Water Directive (DWD) by generating advanced knowledge and developing innovative tools and guidelines for both disinfected and non-disinfected drinking water supply systems. [1]

Within this framework, this study focuses on the development of sustainable nanostructured cellulose-based materials to be deployed for the monitoring of microbiological water quality through the concept of passive sampling. The objective is to design a material capable of capturing potentially pathogenic bacteria present in drinking water distribution networks, without promoting their proliferation, thus ensuring reliable quantification after detachment.

To this end, a series of cellulose-based nanosponges (CNS) were synthesized using TEMPO-oxidized cellulose nanofibers (TOCNF) cross-linked with branched polyethyleneimine (bPEI). [2,3] Different formulations were explored by varying the molecular weight of bPEI (1.8 kDa and 25 kDa).

CNS were evaluated for their ability to capture bacteria (*E. coli* and *Enterococcus)* under controlled conditions. Among the tested materials, CNS prepared with bPEI 1.8 kDa exhibited the most favorable balance between bacterial capture efficiency, preservation of cell viability, suppression of excessive growth, and ease of bacterial release for subsequent quantification.

The performance of this optimized material was also compared with commercial cellulose-based supports, such as cotton gauze, confirming its superior sampling and recovery efficiency.

Overall, these promising results demonstrate the potential of cellulose-based nanosponges, as supporting media for the development of passive sampling devices, promoting green and effective solutions for an effective monitoring in drinking water systems.

This work has received funding from the European Union's Horizon 2020 research and innovation program via the safeCREW project under grant agreement N° 101081980. Call: HORIZON-CL6-2022-ZEROPOLLUTION-01-04.

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POS40

Visible-light generation of aryl radicals from C-X bond in cross-coupling

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The development of metal-free, photocatalyzed aryl-aryl coupling reactions represents a transformative advancement in organic synthesis, driven by the need for sustainable and eco-friendly chemical processes. Biaryl compounds, ubiquitous in pharmaceuticals, agrochemicals, and advanced materials, are traditionally synthesized through metal-catalyzed methods such as Suzuki-Miyaura and Kumada couplings. While these methods are highly efficient, they depend on expensive and often toxic transition metals like copper, nickel or palladium[1]. This reliance on metals introduces environmental concerns, economic challenges, and issues related to metal contamination in the final products.

The use of aryl radicals in organic synthesis has long been limited by the reliance on radical initiators such as Bu_3SnH or AIBN, which present significant drawbacks, including toxicity and limited functional group tolerance. Aryl radicals, known for their ambiphilic nature[2], serve as highly reactive intermediates capable of participating in a wide range of chemical transformations[3]. This strategy leverages their unique reactivity to explore diverse coupling reactions, combining electron-rich or electron-poor partners to construct $C(sp^2)$-$C(sp^2)$ bonds. The versatility of the method lies in its ability to activate aryl halides with unfavorable redox potentials under mild conditions, generating aryl radicals without harsh reagents or metal catalysts. This provides access to a wide array of reactions, expanding the synthetic possibilities of aryl radical chemistry.

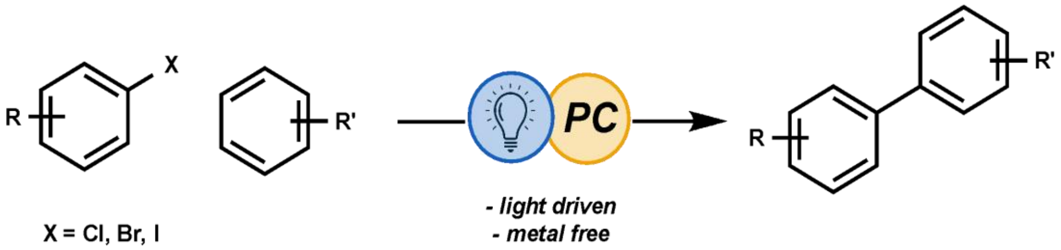

Figure 1: general reaction scheme

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POS41

Enhancing cisplatin efficacy in triple-negative breast cancer through PON2 silencing: insights from FTIRM analysis

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Triple-negative breast cancer (TNBC) represents one of the most aggressive breast cancer subtypes, defined by the absence of estrogen and progesterone receptors and HER2 overexpression [1]. Its high prevalence in younger women and poor response to standard chemotherapy result in unfavorable clinical outcomes [1]. Despite therapeutic advances, TNBC remains difficult to treat due to mechanisms of chemoresistance. Paraoxonase-2 (PON2) has emerged as a factor potentially interfering with cisplatin efficacy by protecting cancer cells from reactive oxygen species (ROS) [1,2]. In this context, PON2 silencing may enhance cisplatin's cytotoxic effect. Fourier Transform InfraRed Microspectroscopy (FTIRM) is a powerful tool for detecting macromolecular alterations in cells post-treatment, thus contributing to the understanding of drug action [2,3]. This study investigates MDA-MB-231 cells with PON2 gene silencing and cisplatin treatment at different time points to (1) elucidate cisplatin's mechanism in TNBC and (2) assess the impact of PON2 silencing on treatment efficacy. MDA-MB-231 cells were transfected with pLKO.1-puro (control; p0) pLKO.1–647 (PON2 silencing; p647), treated with 1 μM cisplatin for 24, 48, and 72 hours and analyzed by MTT assays and FTIRM (4000–900 cm^{-1}, 256 scans, 4 cm^{-1} resolution) spectroscopy. IR data were submitted to multivariate and univariate analyses to detect macromolecular changes induced by treatment.

FTIRM analysis, consistent with MTT data, revealed: (i) decreased DNA, Z-DNA, and RNA, in both p0 and p647, with lower levels in p647 at 24 and 48 hours, suggesting reduced proliferation; (ii) reduced DNA/RNA ratio, and dsDNA/free phosphate ratio, more pronounced in p647, supporting the previous finding; (iii) increased CH_3, with decreased CH_2, indicating shortened lipid chains. These evidence suggested a potential damage to the plasma membrane with an early apoptotic event triggered by cisplatin. Data analysis highlighted a beneficial effect of PON2 silencing within the first 48 hours, while differences at 72 hours were less marked, likely due to excessive cisplatin-induced toxicity masking specific effects of gene silencing.

These preliminary results suggest that PON2 silencing sensitizes MDA-MB-231 cells to cisplatin, particularly in the early treatment phase. The integrated approach, combining biochemical assays, FTIRM, and statistical analyses, provides insights into TNBC chemoresistance and the functional role of PON2. In vitro PON2 silencing emerges as a promising strategy to enhance cisplatin efficacy and potentially improve therapeutic outcomes.

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POS42

NADES-Based Thermosensitive Mucoadhesive Eutectogels for Intranasal Temozolomide Delivery in Glioblastoma

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Glioblastoma multiforme (GBM) represents one of the most critical challenges in modern oncology, due to its aggressiveness and the difficulty of overcoming the blood–brain barrier (BBB) [1]. Temozolomide (TMZ) is one of the first-line drugs used for this pathology; however, it suffers from important drawbacks, including instability in aqueous solutions, resulting in a short half-life [2]. In this work, we propose an innovative thermosensitive mucoadhesive eutectogel, capable of solubilizing and stabilizing TMZ and enabling its intranasal administration to achieve direct brain delivery (nose-to-brain), thereby reducing systemic side effects.The eutectogel combines Deep Eutectic Solvents (DESs) with polymers to obtain high-performance gels while retaining the advantageous properties of DESs [3]. In this study, the DES belongs specifically to the subclass of Natural Deep Eutectic Solvents (NADES), composed of lactic acid and glycerol—two natural, biocompatible substances able to solubilize, protect, and stabilize the active pharmaceutical ingredient, as confirmed by IR spectroscopy. Gelation was achieved using Pluronic F-127, a thermosensitive polymer that ensures sol–gel transition at physiological temperature, facilitating application and prolonged residence in the nasal cavity. To further enhance mucosal adhesion and local retention, hydroxypropyl methylcellulose (HPMC) or medium molecular weight chitosan were incorporated into the matrix.Preliminary carrier characterization studies revealed optimal rheological properties, enhanced long-term drug stability, and achieved a controlled release profile compatible with effective cerebral absorption. This approach represents a promising and sustainable platform for the brain delivery of unstable drugs, offering new therapeutic perspectives for the treatment of brain cancers.

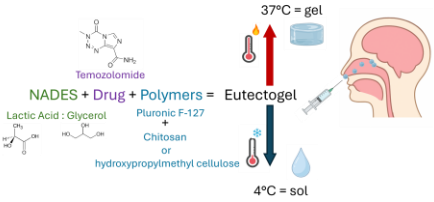

Figure 1: Schematic overview of the eutectogel formulation process.

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POS43

Lipidic autoxidation of ceramides in heterogeneous biomimetic systems

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Lipids are the main constituents of the *Stratum Corneum,* mainly including cholesterol, free fatty acids and ceramides. Each of these undergoes lipidic autoxidation (peroxidation) [1], an autocatalytic free-radical chain reaction responsible for the oxidative destruction of organic molecules and related to oxidative stress, aging, cancer. To counteract this process, antioxidants are necessary. Their development and study are, therefore, key to the design of skin protecting products, along with understanding the skin lipids peroxidation kinetics. Surprisingly, little is known in this regard and current knowledge is only limited to some prototypical model. This work is precisely focused on ceramides autoxidation and the determination of the pertinent kinetic parameters (k_p, k_t and oxidizability) [2]. The selected ceramides are Ceramide NP (or Ceramide 3) and Ceramide EOP (Ceramide 1) and their autoxidation kinetics have been studied using heterogeneous biomimetic systems such as micelles and liposomes, monitoring the oxygen uptake during controlled autoxidation in the presence of well know antioxidants used as references, to determine the kinetic constants. Additional DLS measures have been carried out to characterize the particle's geometry. Autoxidation kinetics of single components is then used to build multicomponent skin-lipid models so to set-up a reference kinetic model to be used in rational antioxidants research.

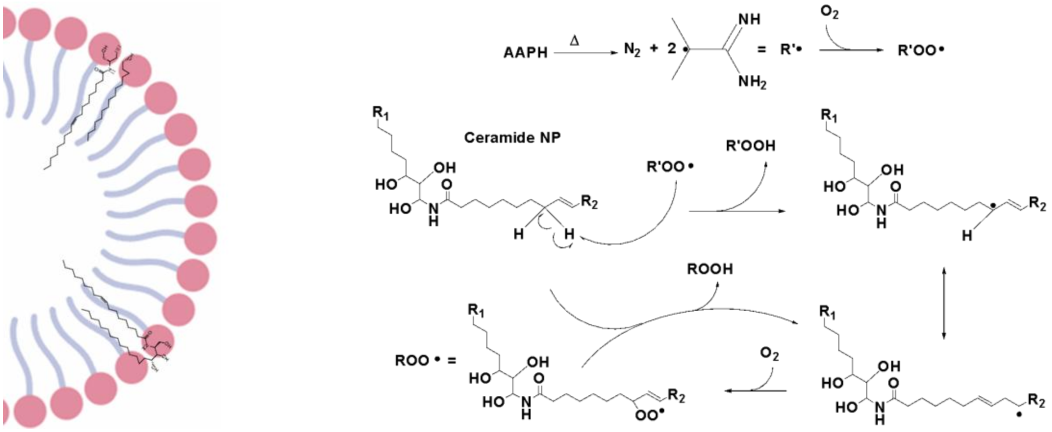

Figure 1: simplified scheme of Ceramide NP autoxidation reaction steps in micelle model.

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POS44

Exploring the Pyrazine scaffold to develop inhibitors towards Casein Kinase 1δ

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Casein Kinase 1δ (CK1δ) is a serine/threonine kinase involved in several biological processes, such as DNA repair, circadian rhythm regulation, Wnt signaling, and neurodegeneration. Due to its involvement in neuroinflammation and neurodegenerative diseases, CK1δ has been identified as a promising therapeutic target for neurological disease tretment3. A drug discovery project started from an in-house screening that identified a pyrazine-based hit-compound displaying an IC_{50} of 1.86 µM towards CK1δ. Structure–activity relationship (SAR) studies were conducted to optimize inhibitory potency by modifying positions 2, 3, 5, and 6 of the core structure. Initial optimization at position 5 with various aryl moieties led to only one active compound in the high nanomolar range. Subsequently, position 3 was explored with a range of substituents—polar, hydrophobic, aryl, alkyl, cyclic, and linear—resulting in several tetrasubstituted compounds with low nanomolar activity and some with good selectivity profiles versus CK1ε. Finally, additional SAR investigations were made at positions 2 and 6 leading to a further optimization in terms of CK1δ inhibition. Most promising derivatives were selected for further studies. Their binding affinities were confirmed using different biophysical approaches, e.g. Thermal Shift Assay (TSA), Microscale Thermophoresis (MST) and Grating-Coupled Interferometry (GCI), which provided Kd values in line with the enzyme activity data. Binding mode at the ATP binding site of these compounds have been investigated through X-ray crystallography, paving the way also to a structure-based hit optimization approach. Considering the Central Nervous System (CNS) as the therapeutic target, compounds were evaluated using Parallel artificial membrane permeability (PAMPA–BBB) assays, revealing moderate to good passive permeability. Cell-based in vitro studies confirmed that the compounds were non-toxic and capable of reducing phosphorylated TDP-43 (pTDP-43) levels, main hallmark of Amyotrophic Lateral Sclerosis (ALS), as reveled by immunoblotting. Further investigation on an in vivo model of Drosophila overexpressing pTDP-43, showed that compounds, besides reducing pTDP-43 levels, improved motor function, and extended lifespan, demonstrating neuroprotective effects. Further characterization, aimed at defining metabolic and selectivity profiles, led to the identification of valuable CK1δ inhibitors that can be used to further investigate the role of this enzyme in neurodegenerative diseases and other conditions, and that can serve as a basis for a hit-to-lead campaign.

POS45

Light-driven semi-hydrogenation of acetylene to ethylene using a cobalt tetraaza-macrocyclic catalyst

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The semi-hydrogenation of acetylene to ethylene is a critical industrial process for producing polymer-grade ethylene, yet conventional thermal catalysis requires H_2 feed, high pressure and temperature, and noble metal catalysts prone to over-hydrogenation to ethane [1]. Light-powered strategies are emerging as promising alternatives [2,3], owing to their potential to directly utilize abundant and sustainable solar energy, but this research is still in its early stages. Here, we report a photocatalytic system for selective acetylene semi-hydrogenation under mild conditions (room temperature, 1 atm) using a non-noble metal cobalt tetraaza-macrocyclic complex ($[Co^{III}(N_4H)Cl_2]ClO_4$) as catalyst, $[Ru(bpy)_3]^{2+}$ as photosensitizer, a sacrificial donor, and a proton source. The system achieves complete acetylene conversion (up to 100%) with >99% selectivity for ethylene and no detectable ethane formation, even under simulated industrial gas streams. This work demonstrates the potential of earth-abundant molecular catalysts for sustainable ethylene purification via light-driven catalysis.

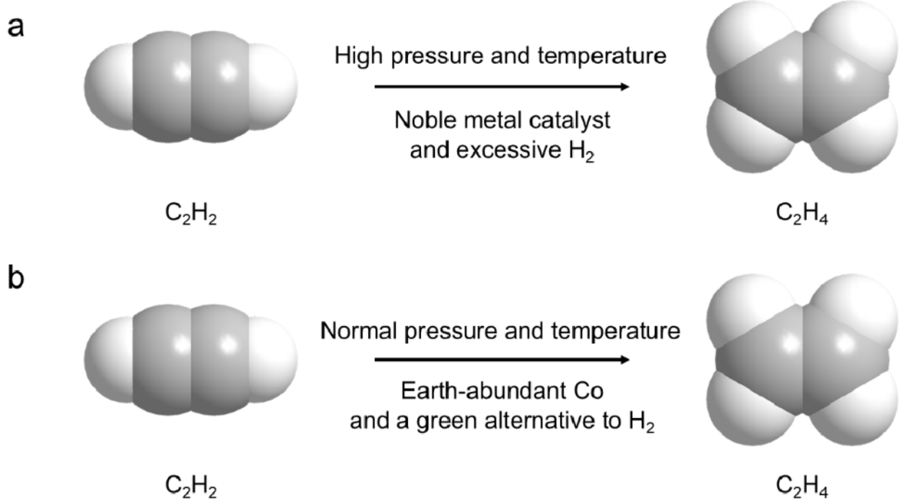

Figure 1: Strategies to produce polymer-grade ethylene. (a) State-of-the-art process for purifying ethylene from acetylene that uses noble-metal catalysts, high temperature and an H_2 gas feed. (b) The photocatalytic approach of this work for the selective conversion of acetylene to ethylene at room temperature by using a cobalt catalyst powered by visible light, in presence of proton sources alternative to H_2.

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POS46

Immuno-affinity electrochemiluminescence detection of viral infections

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The outbreak of coronavirus disease 2019 (COVID-19), caused by the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), has had a profound and unprecedented impact on public health, social behavior, global economy, and individual life [1]. Therefore, in view of the possible occurrence of new challenges, it is highly desirable to develop rapid, accurate and ultrasensitive detection methods for the diagnosis of viruses.

Electrochemiluminescence (ECL) has become a promising analytical technique in immunoassay applications, owing to its superior sensitivity, negligible background signal and easy miniaturization [2]. ECL immunosensors typically utilize luminescent molecule-labeled monoclonal or polyclonal antibody as luminescence probes. However, the limited number of labelable groups and the decrease in binding activity induced by excessive labeling have constrained further improvements in the sensitivity of ECL immunosensors. It is imperative to explore novel antibody molecules that provide more available sites for labeling.

The phage-displayed antibody, as a promising recognition molecule for immunoassay, demonstrates enormous potential in diagnostic applications [3]. Compared with traditional monoclonal or polyclonal antibody, phage-displayed antibody exhibits distinct advantages, including low molecular weight, high quantum yield, remarkable target specificity, strong binding affinity, and excellent stability. Taking advantage of this structural feature to design signal probes for immunoassay enables effective signal amplification, thereby improving the detection sensitivity of the target molecule.

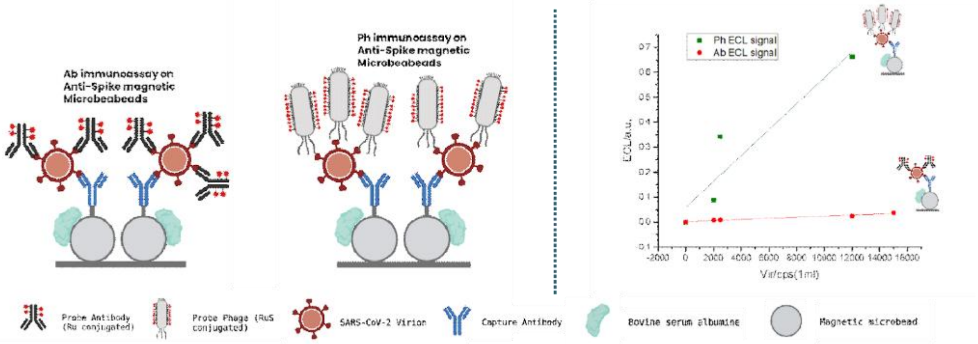

Figure 1: (A) Schematic representation of two different immunoassay assemblies. (B) Comparison of linear relationships between two different immunoassays.

Based on the above research strategy, we constructed an innovative ECL immunosensor for the detection of SARS-CoV-2 by employing phage-displayed antibody as the target recognition element and the specific luminescence probe. The massive viral capsid of phage, which encapsulates the affinity fragment, shows enhanced signal amplification and superior detection sensitivity compared with the double antibody sandwich structure (Figure 1). We remain optimistic about the amplification effect of phage-displayed technology in immunoassay applications.

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POS47

Preliminary evaluation of new sulphur based ligands for ^{103}Pd labelling

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Transition metals cations, particularly soft metal radioisotopes like ^{103}Ag/^{111}Ag, ^{103}Pd, and ^{103m}Rh, exhibit favourable properties for theranostics and targeted radionuclide therapy (TRT). ^{103}Pd is an Auger electron emitter [1], well suited for selective irradiation of single cells or small cell clusters. However, its clinical application is limited due to challenges in developing chelators that ensure in vivo stability and targeting, capable of chelating both parent and daughter radionuclides. This work focuses on the synthesis and validation of three new ligands: CD4S, CDAm3S and AAZ3S (Fig.1) with methylthioethyl pendant arms [2], for stable binding of Pd(II) and its decay product Rh(III).

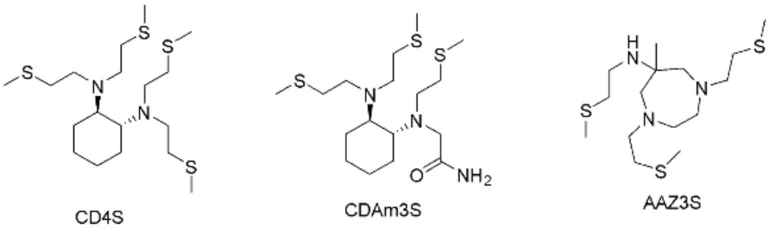
CD4S CDAm3S AAZ3S

Figure 1: Soft ligands synthetized

Pd(II) was used for preliminary complexation studies, monitored by HPLC-MS and UV-Vis spectroscopy. DFT calculations were also performed on both Pd(II) and Rh(III) complexes to evaluate the preferred coordination geometry of the complexes. ^{103}Pd, produced at the Hevesy Laboratory (DTU), was used for radiolabelling. The apparent molar activity at arrival time (AT) was 1.76 MBq/nmol. 2.1 MBq or 4.2 MBq of ^{103}Pd (AT) were added to sodium acetate buffer solution (pH 2.6, 3.8, 4.6) or ammonium acetate buffer (pH 5.5), containing 10 nmol of ligand. Labelling was performed at 80°C or room temperature and monitored by radio-HPLC. At 80°C, CD4S and CDAm3S were able to bind ^{103}Pd quantitatively and at a faster rate than AAZ3S, using low ^{103}Pd concentration. Upon heating, CD4S reached full labelling within 30 minutes in the pH range 2.6–5.5, while CDAm3S required pH between 3.8 and 5.5, and AAZ3S needed pH 3.8 to reach the same result. Experiments are now ongoing for stability, toxicity and labelling improvements (RT labelling, specific activity).

Acknowledgment: This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101008571 (PRISMAP – The European medical radionuclides programme).

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Sponsors talks

SP01 – Roberto Pascucci (Merck)

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SP04 – Cosimo Brondi & Fabio Pizzetti (INSTM)

SP05 – Arianna Massaro & Daniele Del Giudice (EYCN)

SP01

Merck Life Science: who we are and what we do

Roberto Pascucci

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SP02

Biofuels and Green Refinery

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Through the 2023 revision of the Renewable Energy Directive EU/2018/2001, the EU has increased the renewable energy consumption target for member states for 2030 from 32% to 42.5%. In addition, to comply with the directive, member states must require fuel suppliers to ensure that the amount of renewable fuels and renewable electricity supplied to the transport sector leads to a share of renewable energy in final energy consumption in the transport sector of at least 29% by 2030; or a reduction in greenhouse gas intensity of at least 14.5% by 2030 [1]. Eni began working on biofuels back in 2005, when it launched a joint research project with Honeywell UOP focused on innovative biofuels. The collaboration with UOP resulted in the development of a proprietary technology, called Ecofining™, which enables the production of fuels from renewable raw materials. The product obtained through the Ecofining™ process is called HVO (Hydrotreated Vegetable Oil). Eni currently owns three biorefineries operating with Ecofining™ technology. Two are in Italy, in Venice and Gela, and one is in the US, in Chalmette. The first to become operational, in 2014, was the Venice Biorefinery, which was the first traditional refinery in the world to be converted into a biorefinery.

The Ecofining™ process involves two reaction stages. In the first stage, hydrogenation treatment is carried out to saturate the double bonds and remove oxygen. The first stage also promotes the removal of nitrogen, which is a poison for the second-stage catalyst based on noble metals. The product obtained from the first stage is a mixture of paraffins with an excellent cetane number, but poor cold properties. Therefore, the normal paraffins obtained in the first step undergo a second reaction stage in which they are partially converted into their isomers. The purpose of this step is to lower the freezing point and cloud point of the fuel, improving its cold properties. The Ecofining™ process allows to obtain a biofuel free of pollutants, free of oxygen and with superior engine characteristics when compared to fossil diesel or traditional biodiesel. With the Ecofining™ process, it is also possible to obtain sustainable aviation fuels (SAF).

Eni is promoting a business model strongly focused on the circular economy and, regarding Ecofining™, efforts are concentrated on increasing process flexibility, particularly the ability to treat different types of raw materials. The aim is to diversify the feedstocks that can be processed, favoring waste materials such as used cooking oil and agricultural waste and completely avoiding oils derived from crops that could compete with the food supply chain, thus obtaining so-called advanced biofuels.

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SP03

Ten tips for scholarly publishing

Marta Plebani, Monica Azulay

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ACS will present a brief overview of ten tips to improve authors' chances of success when submitting manuscripts.

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Graphics deliver the data in an orderly way and help the reader digest the greatest number of ideas in the shortest amount of time. Be clear and precise, simple but informative, and don't forget to use color!

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SP04

The contribution of academic research in the science and technology of materials: the INSTM network

Cosimo Brondi,[a] Angela Marotta,[a,b] Erika Palazzi,[a,c] Luca Paterlini,[a,d] Fabio Pizzetti,[a,d] and Andrea Caneschi[a,e]

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The INSTM (Italian National Inter-University Consortium for Materials Science and Technology) currently unites 53 Italian universities focused on research in advanced materials and related technologies. This consortium connects a network of over 3000 individuals, including professors, researchers, research fellows, and PhD students. Research areas encompass health sciences, environmental science, nanotechnology, chemical engineering, and materials technology.

INSTM supports research activities within its member universities in the Materials Science and Technology field by offering organizational, technical, and financial assistance. The consortium fosters collaboration by organizing conferences and workshops, funding research fellowships and scholarships, and supporting applications for national and EU grants. It also maintains partnerships and agreements with companies, research institutes, clusters, and innovation hubs across Europe, which will be highlighted.

In 2025, INSTM in collaboration with the Italian Chemical Society (SCI) Young Group, promoted the first *Young Researchers' Forum*, an event developed as a platform for networking and collaboration between the youngest members of both the INSTM consortium and SCI, who specialize in Materials Science, Technology, and Chemistry in its various branches.

Figure 1: Group photo of the INSTM Young Researchers' Forum 2025

SP05

Building bridges for young chemists: a journey through the European Young Chemists' Network (EYCN)

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The idea for the European Young Chemists' Network (EYCN) within EuChemS was first conceived during a series of young chemists' meetings in Europe. The network was founded in 2006 with a key document titled "*Aims, Tasks and Goals of EYCN*" written at the 1st European Chemistry Congress in Budapest. The following year, representatives from various societies were invited to Berlin to formalize the EYCN's structure, and within just three weeks the EuChemS Executive Committee approved the new statutes, officially recognizing the EYCN as the youth division of EuChemS.

Nowadays, the EYCN represents young members from any EuChemS member society, based on their national criteria. Each young member of a chemical society which is part of EuChemS automatically becomes part of the EYCN. Today, the EYCN has delegates and representatives in 22 countries (from 25 chemical societies). The EYCN's mission is to advance the field of chemistry in Europe while providing educational and networking opportunities for students and professionals. EYCN delegates work in 5 teams being Communication, Network, Global connection, Science and Membership (Figure 1). Nowadays, there are four Italian delegates in EYCN. EYCN promotes various awards at conferences, organizes Career Days to develop soft skills, and supports exchange programs to enhance member mobility. To achieve these goals, the EYCN collaborates with industrial partners and other global young scientific societies.

EuChemS
European Chemical Society
—European Young Chemists' Network—

Our mission

Connecting and Empowering Young Chemists across Europe

How do we achieve it?

- Representation of young chemists at the European level
- Collaboration with the European Institute for Industrial Leadership (EIIL)
- Soft skills and career development workshops
- Scientific conferences, events (*EYCheM, EuChemS Chemistry Congress*)
- Science communication competitions (*Photochimica, Video Competition*)
- Diversity, inclusion, and sustainability initiatives (*Green Chem, Women in Chemistry*)
- E-learning courses

Who are we?

40+ national chemistry societies
45.000+ young chemists
Early-career professionals, postdocs, PhD candidates and **STUDENTS**

Follow us

Contact us:
chair@eycn.eu

Meet our Teams

Membership

- Establishing new contacts with chemical societies joining EYCN
- Chemistry Across Europe
- EYCN Alumni
- EYCN website

Networks

- Workshops, webinars
- Science Policy
- Mental Health and Diversity
- How are young Chemists doing?
- Mentoring and Excellence Initiatives

Science

- Scientific podcast
- "Photochimica" + "Chemistry Rediscovered" contests
- "What should stick?" - introducing important research topics in sticky note-format

Global Connections

- Fostering connections with chemical societies outside Europe
- Internal cooperation
- Discovering worldwide perspectives: Eurospectives, Glospectives

Communication

- Monthly newsletter
- Highlighting EYCN activity: LinkedIn, Instagram, YouTube
- "EYCN Career Compass", informing about academic job opportunities

We unite **We empower** **We inspire**

Figure 1: EYCN poster (https://www.euchems.eu/divisions/european-young-chemists-network/).

List of Participants

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Società Chimica Italiana

Società Chimica Italiana (SCI) is a scientific association that includes more than 6000 members. It was founded in 1909 and erected as a Legal In stitution with R.D. n. 480/1926. SCI members carry out their activities in universities, public and private research institutes, schools, industries, or as freelancers. They are joined not only by the interest in chemical sciences, but also by the desire to contribute to the cultural and economic growth of the national community, within a global framework, improving the quality of human life and the protection of the environment. SCI is organized in Divisions and Sections: Divisions are thematic branches, gathering members working in the same field or sharing the same scientific interests; Sections are local branches, gathering people working or living in the same territory.

For new members

All the participants to the *Merck Young Chemists' Symposium XXIV edition* are (or are going to be) SCI members. Those who were not yet SCI members before the conference, must fill the request form included in the Conference bag in order to complete the membership procedure. Those who chose the 1-year subscription will be enrolled until 31/12/2025; those who chose the 2-year subscription will be SCI members up to the end of 2026.

SCI Giovani / SCI Young

All SCI members younger than 35 years old belong to SCI Giovani, an interdisciplinary group organizing multiple initiatives precisely devoted to youngers, such as prizes, workshops, and the very congress you are attending.

You can find all the information about these activities on our website
https://www.soc.chim.it/sci_giovani/home

as well as on our social media pages

@SCI Giovani

We strongly suggest to actively take part to the initiatives proposed by SCI Giovani, since they constitute a fundamental opportunity to familiarize with the national and international scientific community, to experience new opportunities of personal and professional growth.