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Sezione Sicilia

Università degli Studi di Messina

Società Chimica Italiana
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Atti del

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delle Sezioni Sicilia e Calabria
della Società Chimica Italiana

Messina, 2-3 dicembre 2024
Polo Papardo UniMe
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Programma

Lunedì 2 dicembre

Sessione mattutina Aula Magna "Vittorio Ricevuto"

8.30-9.30	Registrazione
9.30-10.00	Saluti Istituzionali

Sessione I Chairs: Cosimo Gianluca Fortuna (UniCT) ed Angela Malara (UniRC)

10.00-10.30	PL1 – Maria Grazia Musolino (UniRC) – Can more disorder be better? From high-entropy materials basic concepts to applications
10.30-10.45	OC1 – Chiara Alessandrello (UniRC) – Novel nanostructured electrocatalysts for GREen hydrogEN production via water electrolysis based on High-Entropy Materials (HEM4GREEN project)
10.45-11.00	OC2 – Erika Saccullo (UniCT) – From Waste to Resource: A Polysaccharide-Based Composite for Converting VOCs into Valuable CO_2-derived Products
11.00-11.15	OC3 – Dario Perziano (UniCAL) – Green synthesis of core/shell Iron oxide/Gold nanoparticles for Pb^{2+} sequestration in water
11.15-11.35	**Coffee Break**

Sessione parallela (SBA-T-2A)

Sessione II Chairs: Maria Rosaria Plutino (CNR-ISMN, ME) e Mario Prejanò (UniCAL)

11.30-13.30	Contest ChiMiCapisce

Sessione II Chairs: Mariagrazia Fortino (UniCZ) e Daniela Iannazzo (UniME)

11.35-12.05	PL2 – Graziana Messina (UniCT) – Smart Active Biointerfaces
12.05-12.20	OC4 – Giovanna Li Petri (CNR-ISMN, PA) – Advancing SilverSil Sol-Gel Chemistry Towards Novel Antibacterial Coatings for Practical Applications
12.20-12.35	OC5 – Lidietta Giorno (CNR-ITM, CS) – Tuning membrane properties for enzyme heterogenization
12.35-12.50	OC6 – Elena Giuliano (UniCZ) – Poloxamer- and Poloxamine-based Multifunctional Hydrogels as Advanced Drug Delivery Systems
12.50-13.05	OC7 – Martina Maria Calvino (UniPA) – Geopolymeric Films based on halloysite clay nanotubes for environmental applications
13.05-13.10	FC1 – Giuseppe Cinà (UniPA) – Development of nanomaterials based on halloysite as carrier for cIDPR molecules and PNA
13.10-13.15	FC2 – Roberto Di Pietro (UniME) – A Comparative study of Two MIL-100(Fe) MOFs Synthesized via Conventional and Green Methods for Water Harvesting
13.15-13.20	FC3 – Federica Meringolo (UniCAL) – Cellulose matrices amination towards the preparation of antimicrobial composites
13.20-13.25	FC4 – Veronica Ciaramitaro (UniPA) – Polysaccharide-based film for a controlled release of indocyanine green for biomedical applications
13.25-13.30	FC5 – Simona Crispi (CNR-IMM, CT) – Ion exchange membranes for wastewater treatment
13.30-14.45	**Light lunch e sessione poster**

Sessione pomeridiana 1 (Aula Magna "Vittorio Ricevuto")

14.45-15.00	Saluti del presidente della SCI Gianluca Maria Farinola

Sessione III Chairs: Ugo Perricone (Fondazione RiMed) e Pierluigi Plastina (UniCAL)

15.00-15.30	PL3 – Michele De Luca (UniCAL) – Chemometric Tools in Pharmaceutical Analysis: Multivariate Curve Resolution-Alternating Least Squares (MCR-ALS) for Analysing Complex Chemical Systems
15.30-15.45	OC8 – Gianfranco Cavallaro (UniCT) – In silico design and synthesis of new potential antibacterial drugs and ligand-protein interaction studies for new active molecules against COX-1 receptor
15.45-16.00	OC9 – Maria Antonietta Occhiuzzi (UniCAL) – Structure-based drug design and virtual ligand screening for the discovery of GPER targeting compounds
16.00-16.15	OC10 – Maria Dichiara (UniCT) – Discovery and structure-based optimization of potent sigma receptors ligands
16.15-16.30	OC11 – Fortuna Ponte (UniCAL) – Innovative Approaches in Oncology: Insights from Density Functional Theory on PACT Mechanisms
16.30-16.45	OC12 – Giovanni Bella (UniME) – Vibrationally-resolved deep-red circularly polarized luminescence spectra of C70 derivative through gaussian curvature analyses of ground and excited states
16.45-17.00	**Coffee Break**

Sessione IV Chairs: Delia Chillura Martino (UniPA) e Tiziana Marino (UniCAL)

17.00-17.15	OC13 – Luca Calantropo (UniCT) – Photo-thermocatalytic CO2 methanation on SiC/hydrotalcites-derived catalysts
17.15-17.30	OC14 – Elisabetta Grazia Tomarchio (UniCT) – Designing of a Monolithic Photo-Fenton Catalyst from a Fungal Hydroxypyrone Derivative
17.30-17.45	OC15 – Marco Francesco Torre (UniME) – Ammonia synthesis via plasma-assisted electrochemical nitrogen conversion at ambient conditions
17.45-18.00	OC16 – Narimene Aoun (UniPA) – Composite photocatalysts prepared with materials from spent Li-ion batteries and g-C3N4 for the photoreforming of organics in aqueous solution to obtain H2
18.00-18.05	FC6 – Giuseppe Angellotti (CNR-ISMN, PA) – Essential Oils in Sustainable Agriculture: Sol-Gel Microencapsulation for Prolonged Insecticidal Efficacy
18.05-18.10	FC7 – Beatrice Russo (CNR-ITM, CS) – Plastic pollution: Membrane Separation and Photocatalysis for the treatment of water effluents
18.10-18.15	FC8 – Stefano Scoditti (UniCAL) – Mechanistic Insights into the Reduction Process of Pt(IV) Complexes: From G-Quadruplex Binder Activation to Riboflavin-Mediated Photocatalysis
18.15-19.30	Assemblea dei soci Sezione Sicilia
20.30-23.30	**Cena sociale presso "Il Grecale"**

Sessione pomeridiana 2 (SBA-T-2A)

Sessione V Chairs: Emilia Furia (UniCAL) e Gabriele Lando (UniME)

15.35-15.50	OC17 – Mariosimone Zoccali (UniME) – The usefulness of the cryogenic zone compression gas chromatography-mass spectrometry approach for analysis of polycyclic aromatic hydrocarbons in food
15.50-16.05	OC18 – Giuseppe Nocito (CNR-ISMN, ME) – An integrable sensoristic platform for β-amyloid based on supramolecular interactions
16.05-16.20	OC19 – Giuseppe Proietto Salanitri (CNR-IPCB, CT) – Macroporous Porphyrin Cryogels: High-Efficiency Mercury Adsorption and Colorimetric Sensing
16.20-16.25	FC9 – Emanuele Luigi Sciuto (UniME) – Pathogen nucleic acid electrochemical detection for PCR-free sensing application
16.25-16.30	FC10 – Roberta Farina (CNR-IMM, CT) – Electrochemical sensors for nitrate and ammonia ions detection in water
16.30-16.35	FC11 – Emanuele Zanda (UniME) – Enhancing the photoluminescence of citrus-derived Carbon Quantum Dots through Experimental Design

16.35-16.40	FC12 – Silvia Orecchio (UniPA) – Metal release from perovskite solar cells: environmental risk assessment by voltammetric analysis
16.45-17.00	Coffee Break

Sessione VI Chairs: Donatella Aiello (UniCAL) e Maria Rosaria Plutino (CNR-ISMN, ME)

17.05-17.20	OC20 – Davide Lascari (UniPA) – Turning local waste into resource: Opuntia ficus-indica cladodes and Prunus dulcis husk as adsorbents of lead ions
17.20-17.35	OC21 – Federica Curcio (UniCAL) – Nanoformulations of cosmetic interest for the cutaneous uptake of nickel
17.35-17.50	OC22 – Valeria Loise (UniCAL) – Expanding SUPRADES beyond cyclodextrins: preparation and study of resorcin[4]arene/choline chloride binary system
17.50-17.55	FC13 – Carmen Lo Sardo (UniCAL) – An eco-friendly analytical approach for lithium battery recycling
17.55-18.00	FC14 – Maria Francesca Baratta (UniCAL) – Sulfur-Functionalized Single-Walled Carbon Nanotube Buckypaper/MTV-BioMetal−Organic Framework Nanocomposites for Gold Recovery
18.00-18.05	FC15 – Chiara La Torre (UniCAL) – Nutritional profile and antioxidant capacity of plant-based kefir milks
18.05-18.10	FC16 – Giulia Itri (UniRC) – Recovery of spent lithium ion batteries for catalytic biomass upgrading
18.10-18.15	FC17 – Ilaria Citro (CNR-IPCF, ME) – Harnessing Nanotechnology: Boosting Solar Cell Performance with Quantum Dots and Gold Nanoparticles
18.15-19.30	Assemblea dei soci Sezione Calabria

Martedì 3 dicembre

Sessione mattutina Aula Magna “Vittorio Ricevuto”

Sessione VII Chairs: Laura De Luca (UniME) e Raffaella Mancuso (UniCAL)

09.00-09.30	PL4 – Barbara Parrino (UniPA) – Development of 3-amino-1,2,4-triazine derivatives as selective PDK1 inhibitors: synthesis and biological insights in pancreatic ductal adenocarcinoma
09.30-09.45	OC23 – Elsa Calcaterra (UniME) – Development of Peptide-Based SARS CoV-2 Mpro/hCatL Dual Inhibitors as Antiviral Agents
09.45-10.00	OC24 – Roberta Bivacqua (UniPA) – Thiazole-based compounds as promising fusion inhibitors of influenza A/H1N1 virus
10.00-10.15	OC25 – Luisa D’Anna (UniPA) – Asymmetric Salphen Complexes and Selective Targeting of G-Quadruplex Structures
10.15-10.30	OC26 – Ana Laura Coria Gutierrez (UniME) – Development of Drug Delivery Systems based on MagnetoCyclodextrins for osteosarcoma treatment
10.30-10.45	OC27 – Giuliana Costanzo (UniCT) – Design, synthesis, and biological evaluation of new ligands as potential therapeutic agents for persistent pain treatment
10.45-11.00	OC28 – Patrizio Russo (UniCAL) – New Synthesis of 2-(Benzofuran-2-yl)acetamides
11:00-11:05	FC18 – Giuseppe Cosentino (UniCT) – Evaluation of tetrahydropyrrolo[3,4-c]pyrazole derivatives as sigma-1 receptor ligands
11:05-11:10	FC19 – Giulia Culletta (UniPA) – Rescuing P53 by new translational readthrough inducing drugs
11:10-11:15	FC20 – Antonella Di Francesco (UniCT) – Preliminary Results about the Structural Characterization of Chickpea β-chain Legumins: An integrated Bottom-up and Top-down proteomic approach

11.15-11.30 Coffee Break

Sessione VIII Chairs: Francesca D'Anna e Agostino Marrazzo

11:30-11:45	OC29 – Marco Milone (UniME) – H-bonding solvents influence on the conformation adopted by a novel calix[4]tube both in liquid and in solid phase
11.45-12.00	OC30 – Giovanna Raia (UniPA) – Upcycling polycarbonate waste: an efficient alternative to disposal
12.00-12.15	OC31 – Antonella Buccafuri (UniCAL) – Phenolic fraction and antioxidant activity of Palm oil
12.15-12.30	OC32 – Giuseppina Cacciatore (UniCAL) – Differential proteomics approach to investigate human aging
12.30-12.35	FC21 – Maura Monforte (UniME) – Bolaamphiphiles via sulfenic acid
12.35-12.40	FC22 – Maria Marra (UniCAL) – Chirality influences the biological properties of novel NHC-gold and -silver complexes
12.40-12.45	FC23 – Mariangela Novello (UniCAL) – Oxidative carbonylation of β-amino alcohols catalyzed by Pd supported on silica-POSS-Imi
12.45-12.50	FC24 – Maria Gaetana Giovanna Pittalà (UniCT) – Structural characterization of the protein fraction extracted from extracellular vesicles secretes by astrocytes using high-resolution mass spectrometry
12.50-13.30	Premiazioni e saluti

Plenarie

PL1

Can more disorder be better? From high-entropy materials basic concepts to applications

Maria Grazia Musolino*

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The development of new and advanced materials, characterized by versatile but tailorable properties as well as improved environmental compatibility is one of the greatest challenges faced by the scientific community for fulfilling the needs of the constantly evolving modern and more sustainable technology and breakthroughs in the future. Towards this direction, a new concept to materials design based on the high-entropy approach has emerged in recent years, becoming one of the hot trends in the field of materials science. The application of this concept has led to development of a wide class of intriguing materials, so called high-entropy materials (HEMs), with outstanding physical and chemical properties, starting with high-entropy alloys (HEAs), introduced for the first time and independently by the studies of Cantor et al.[1]and Ye et al.[2] in the 2004.

HEMs consist of multiple principal elements (typically, five or more elements) in equimolar or close to equimolar ratios, which are randomly distributed in one homogenous single phase structure of solid solutions driven by high configurational entropy. Among HEMs, high-entropy oxides (HEOs) are very appealing nanomaterials for the possibility of obtaining amazing properties, by exploiting a great number of possible elemental combinations, making them potentially suitable for a wide range of applications, including energy storage, large-k dielectric materials, water splitting, catalysis, thermal protection and insulation.

In this talk, a general overview of high-entropy materials will be presented with particular focus on the HEOs, concerning not only their synthesis and characterization but also their functional properties as well as practical applications. Finally, some examples of our present research are reported[3,4].

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[4] C. Triolo, S. Santangelo, B. Petrovičovà, M. G. Musolino, I. Rincón, A. Atxirika, S. Gil, Y. Belaustegui Appl. Sci. 2023, *13*, 721.

PL2

Smart Active Biointerfaces

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Smart active interfaces have attracted a huge research interest in the last decades, owing to their action as multifunctional, self-regulating and pluripotent building blocks for innovative technologies and advanced devices. In turn, smart materials become able to sense and respond to external stimuli, adapting their properties and functions accordingly.

Among smart and active interfaces, biointerfaces have shown remarkable advancements driven by the convergence of materials science, biology, and nanotechnology. Active smart surfaces obtained by applying different surface modification strategies can modulate biomolecule activity, protein immobilization, driving in turn important biological processes like cell adhesion and migration at the liquid–solid interface and they can be extremely useful in diverse biological and medical applications. In this context, the study of protein adsorption at solid-liquid interface is of crucial relevance in biomaterial and healthcare applications. The role of suitably engineered surfaces, built by functionalizing the substrate with specific and density-controlled anchoring sites enabling the formation of stable and uniform layer of protein molecules for bio-application will be presented.

Moreover, a detailed characterization of the interaction between proteins and surfaces will be provided, by analysing the surface properties effect induce by protein adsorption.

Additionally, in the context of smart materials, conductive polymers have emerged in recent years as promising materials in the field of bioelectronics and tissue engineering due to their interesting mixed ionic-electronic conductivity, biocompatibility, and tunable physico-chemical properties. The biological response, in terms of osteoconductivity and osteoinductivity, of human adipose-derived mesenchymal stem cells cultured at interfaces have been studied, showing a good response to induce osteogenic differentiation of osteoprogenitor cells, even in absence of specific inductive growth factors, being thus a promising strategy for bone regenerative medicine.

Therefore, the development of new active smart biointerface able to drive the protein orientation and anchoring and the cell response represents the main challenge in the field of biomedical application.

PL3

Chemometric Tools in Pharmaceutical Analysis: Multivariate Curve Resolution-Alternating Least Squares (MCR-ALS) for Analysing Complex Chemical Systems

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Chemometric methodologies play a pivotal role in modern pharmaceutical analysis, providing the tools necessary to extract valuable information from complex experimental datasets. Among these, Multivariate Curve Resolution – Alternating Least Squares (MCR-ALS) stands out as a particularly powerful technique for analysing intricate chemical systems where overlapping signals, mixtures, or hidden information make traditional analysis methods inadequate.

MCR-ALS decomposes the data, such as spectroscopic or chromatographic data, into their underlying components without requiring prior knowledge of the system (Fig.1). This algorithm enables the evaluation of the concentration profiles and pure spectra of the different species in a sample, offering insights into the chemical behaviour of pharmaceutical matrices under various conditions[1]. One key advantage of MCR-ALS is its flexibility; it can handle data from multiple experiments and across diverse analytical techniques such as UV-Vis, HPLC-DAD, mass spectrometry, and others, improving the resolution of complex systems and minimizing ambiguities. In pharmaceutical research, MCR-ALS is invaluable for studying drug stability, degradation pathways, interaction with excipients, and even biopharmaceutical processes. The technique is particularly effective in identifying unknown degradation products, estimating kinetic rates, and optimizing formulations by providing a clear understanding of how the components in a mixture evolve over time[2].

$$\mathbf{D} = \mathbf{C}\,\mathbf{S}^{T} + \mathbf{E}$$

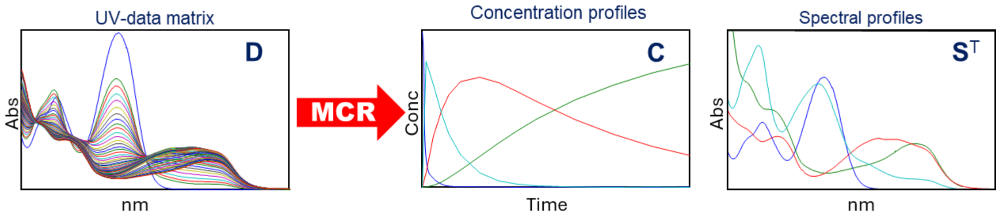

Figure 1. MCR-ALS results.

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[2] M. De Luca, G. Ioele, F. Grande, S. Platikanov, R. Tauler, G. Ragno *Journal of Pharmaceutical and Biomedical Analysis* **2020**, *186*, 113332

PL4

Development of 3-amino-1,2,4-triazine derivatives as selective PDK1 inhibitors: synthesis and biological insights in pancreatic ductal adenocarcinoma

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Deregulation of cellular metabolism is a critical hallmark of cancer, significantly contributing to cancer progression and resistance, particularly in aggressive types like pancreatic ductal adenocarcinoma (PDAC), one of the main aggressive types of cancer, characterized by late prognosis and drug resistance.[1] Pyruvate dehydrogenase kinases (PDKs) play a vital role in metabolic regulation, and their overexpression is often observed in various cancers, including PDAC.[2] Although a few PDK inhibitors have been reported, their structural diversity presents opportunities for new therapeutic developments.[3]

To identify novel PDK inhibitors, we utilized a molecular hybridization approach that combines multiple active scaffolds into single molecules. Thus, we synthesised new hybrid compounds that merge different pharmacophoric sub-units such as 1,2,4-amino triazines, 7-azaindoles, and indoles.

The resulting derivatives demonstrated strong antiproliferative effects against pancreatic cancer cells in both 2D and 3D culture models with IC_{50} values ranging from low- to submicromolar level. Moreover, they exhibited potent inhibition of PDK1 and PDK4 enzymatic activities, confirmed by docking studies, exhibiting for PDK1 IC_{50} values more potent than the well-known reference inhibitor, dichloroacetate (DCA).

Mechanistic studies indicated that these derivatives disrupt the PDK/PDH axis, leading to metabolic and redox impairment, ultimately triggering apoptosis in cancer cells. *In vivo* studies in murine models of highly aggressive Kras-mutant tumors showed that the most promising compound, effectively targeted the PDK pathway, reducing tumor growth while maintaining body weight, demonstrating superior tolerability compared to traditional chemotherapeutics like cisplatin and gemcitabine.

As a proof of concept, additional studies confirming the potential of the new library as PDK1 inhibitors will be presented and discussed.

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Comunicazioni orali

OC1

Novel nanostructured electrocatalysts for GREen hydrogEN production via water electrolysis based on High-Entropy Materials (HEM4GREEN project)

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Currently, alkaline water electrolysis (AWE) powered by renewable sources is one of the least costly and green technologies to produce hydrogen.

The project “HEM4GREEN” (High-Entropy Materials as cost-effective catalysts in anion exchange membrane water electrolysis for GREen hydrogEN production) is focused on the development and engineering of novel nanostructured electrocatalysts based on high-entropy materials[1] (HEMs). Its goal is to develop cost-effective, efficient and critical raw materials-free HEM-based catalysts for oxygen and hydrogen evolution reactions, to be used in an electrolyzer employing a polymeric anion exchange membrane[2] (AEM) as the electrolyte.

HEMs are prepared by scalable techniques, suitable for mass-production; HEM-based electrodes are fabricated by ink spraying and assembled in a zero-gap AWE full cell, which is electrochemically tested.

The entire value chain will be examined, namely: i) studying new electrode materials; ii) fabricating and assembling electrodes for AEM electrolyzers; and iii) achieving a current density of 1 A/cm^2 at a potential of 2 V at the temperature of 50°C, with a single cell degradation rate below 5-7 µV/h (i.e. approximately 0.2-0.4% per 1000 h) at 1 A/cm^2.

The results achieved in the first two quarterlies will be presented.

The Authors gratefully acknowledge the European Union for the financial support to this project through Next-Generation EU funds (National Recovery and Resilience Plan, PNRR - Mission 4 “Education and Research” - C2 component - Investment 1.1, Fund for the National Research Program and Projects of Relevant National Interest, PRIN).

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OC2

From Waste to Resource: A Polysaccharide-Based Composite for Converting VOCs into Valuable CO_2-derived Products

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This study presents a sustainable and innovative natural material synthesized by grafting alginic acid,[1] a polysaccharide abundantly found in brown algae, with a xanthine derivative. The resulting material was then conjugated with magnetite (Fe_3O_4) (Figure 1). FT-IR and NMR spectroscopy confirmed the functionalization of the composite, while TGA assessed thermal stability. SEM-EDX provided valuable insights into the material's morphology, and XPS was employed to study its surface properties. The incorporation of magnetite serves a dual purpose: 1) It facilitates the photoconversion of volatile organic compounds (VOCs),[2] such as toluene, into CO_2, and 2) it enables the magnetic recovery of the catalyst, making the process more efficient. The catalytic activity is primarily attributed to the organic portion (AX), which can convert CO_2 into valuable synthetic products like carbonates. Combining organic (AX) and inorganic (Fe_3O_4) components, this unique dual-functionality allows the material to transform pollutants like VOCs into CO_2 and subsequently into reusable compounds like carbonates. Moreover, due to its natural origin, this material represents a promising green solution to address environmental challenges, offering a sustainable approach to pollution mitigation and resource recovery.

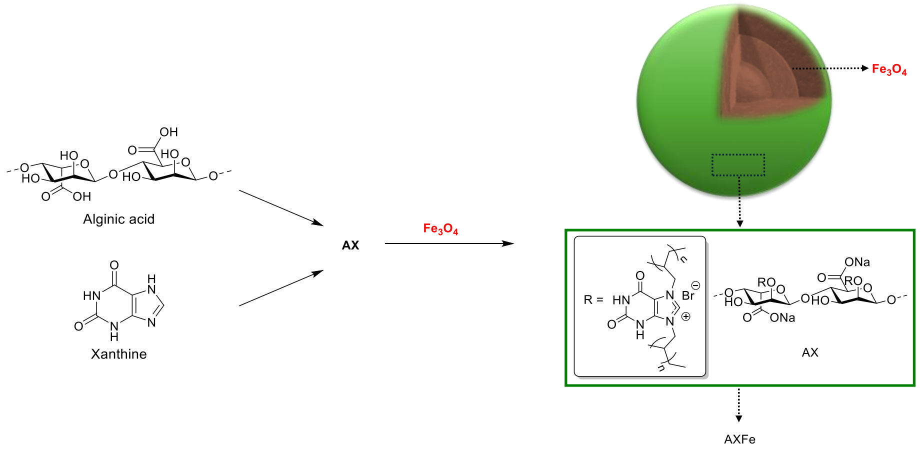

Figure 1. Scheme for the preparation of AX and AXFe materials.

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OC3

Green synthesis of core/shell Iron oxide/Gold nanoparticles for Pb^{2+} sequestration in water

Dario Perziano,[1*] Antonio Tagarelli,[1] Rosangela Elliani,[1] Oriella Gennari [2] and Massimo La Deda,[1,2]

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Increased human and industrial activities have led to a progressive reduction in the availability of drinking water, aggravated by contamination by heavy metals such as Lead (Pb^{2+}). Heavy metals can accumulate in organisms, causing serious health problems. [1] In particular, Lead, present in water due to obsolete pipes, is a powerful neurotoxin that causes neurological and systemic damage, especially in children.[2]

To address this issue, various methods have been developed to remove lead from water, such as membrane filtration, adsorption, and the use of biopolymers and Metal-Organic Frameworks (MOFs).[3] In an attempt to find an efficient and eco-friendly method to sequester Lead present in water, here we present the use of gold nanoparticles (AuNPs), functionalized with a magnetic core (Fig 1a) and synthesized using aqueous extracts of a local plant growing in Sila mountains (Fig 2b). This eco-friendly approach offers an innovative and green solution compared to traditional MOFs, overcoming the challenges related to their stability and scalability.

The synthesized gold nanoparticles, with their large surface coated with anthocyanins and caffeic acid derivatives, effectively bind lead ions via electrostatic interactions, and the presence of iron oxide (Fe_3O_4) nuclei allows for easy removal of the nanoparticles from the treated water by a magnetic field, ensuring effective remediation and the possibility of reusing the nanoparticles.

The synthesis of these nanoparticles uses local resources and an eco-sustainable process. Plant extracts, rich in redox-active compounds, act as reducing and stabilizing agents, avoiding the use of cad substances with a high environmental impact. After use, the nanoparticles can be recovered, regenerated and reused, making the process sustainable in the long term.

This approach not only addresses the problem of lead contamination in drinking water, but also represents a significant step towards water treatment technologies aligned with the principles of the circular economy and environmental sustainability.

OC4

Advancing SilverSil Sol-Gel Chemistry Towards Novel Antibacterial Coatings for Practical Applications

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Organically modified silicates (ORMOSIL) are hybrid materials derived from the hydrolytic polycondensation of silanes modified with organic groups, combined with traditional alkoxide precursors.[1] Especially when doped with organic molecules or metal nanoparticles, these functional materials are of significant interest across various fields, including optics, electronics, energy, environmental science, and biomedicine.[2] Among the various microencapsulation technologies, the sol-gel entrapment of metal nanoparticles (NPs) in ORMOSIL matrices offers distinct advantages, including enhanced physicochemical stabilization of the NPs and the ability to form doped materials in various forms, such as powders, films, thin coatings, and monoliths, making it versatile for multiple applications.[3]

Introduced in 2020, SilverSil is an innovative sol-gel material that incorporates silver nanoparticles (AgNPs) within an ORMOSIL matrix, offering broad-spectrum *in vitro* antibacterial activity.[4] In this lecture, I will present the development of new SilverSil materials obtained through a two-step sol-gel hydrolytic polycondensation process of tetraethyl orthosilicate (TEOS) and organically modified silanes methyltriethoxysilane (MTES) and (3-aminopropyl)trimethoxysilane (APTMS) in the presence or without different concentrations of $AgNO_3$. The effects of selected parameters including the water/alkoxide ratio, the absence of ethanol as a co-solvent, the time of gel aging, and the alcogel/hydrogel drying conditions on the resulting SilverSil materials were investigated.[5] Initial findings are promising and suggest excellent antibacterial efficacy against both gram-positive and gram-negative bacterial strains for all Ag-doped powders. When deposited on fabrics, like cotton and PET, SilverSil provides textiles and produce stable garments with long-lasting antibacterial protection, making them useful for medical applications, clothing, or any other field requiring antimicrobial finishes.

Acknowledgements

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OC5

Tuning membrane properties for enzyme heterogenization

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The attachment of enzymes to synthetic membranes proved to enhance enzyme stability. Furthermore, membranes can compartmentalize phases and govern mass transport. Therefore, they can perform simultaneously the catalytic conversion and the separation of reaction products, which leads to a high conversion rate based on Le Chatelier’s principle. On the other hand, to achieve high catalytic performance, the heterogenization process and the microenvironment conditions must be carefully tuned. The lecture will illustrate the influence of the type of membrane (material, structure, charge, wettability), type and amount of immobilized enzyme, and nature of reagent(s) on the observed catalytic properties as well as the influence of fluid dynamic conditions on the enzyme-loaded membrane reactor performance. Case studies using hydrolase enzymes to produce high-added value components, including optically pure enantiomers, will be discussed. Since communication at the molecular level is governed by chiral interaction, technologies able to produce optically pure enantiomers are highly demanded. The lecture also attempts to analyze the drivers and brakes of the technology and the rejuvenated perspective in sustainable biorefinery.

OC6

Poloxamer- and Poloxamine-based Multifunctional Hydrogels as Advanced Drug Delivery Systems

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Hydrogels are hydrophilic networks capable of retaining large amounts of water or biological fluids. While they offer advantages like biocompatibility, low toxicity, and similarity to the extracellular matrix, their implantation requires invasive surgery, causing patient discomfort. Thermosensitive hydrogels address these issues by being administered in liquid form and then undergoing gelation in the body, allowing for sustained drug release, reducing dosing frequency, and enhancing patient compliance. Poloxamers and poloxamines, made up of poly(propylene oxide) (PPO) and poly(ethylene oxide) (PEO) units, are the most widely used materials for the production of these advanced drug delivery systems[1,2].

Our research team showed that poloxamer 407 (P407)-based hydrogels can be used for *in situ* administration of rutin, a plant-derived flavonoid with various pharmacological effects but low bioavailability due to poor water solubility. P407 is a linear tri-block copolymer made up of a central PPO block flanked by two hydrophilic PEO units. The hydrophobic domains within the structure help the retention of poorly water-soluble molecules in the polymeric network. The addition of rutin to P407 solutions (20%, w/w) did not affect the physico-chemical properties of the resulting hydrogels at drug concentrations up to 0.1% w/w, suggesting that the drug can be taken without co-solvents to avoid potential side effects[1]. *In vitro* scratch assay on human keratinocytes demonstrated that the association of the flavonoid with P407 provides a noteworthy increase of cell proliferation compared to the single components. Moreover, the formulation promoted a better cutaneous wound healing in rats compared to the free drug and the commercial wound dressing DuoDERM®, providing the rationale of using the proposed system for the treatment of skin injuries.

Poloxamine 908 (P908) is an X-shaped amphiphilic block copolymer consisting of an ethylenediamine core linked to four PPO-PEO chains. Aqueous solutions of P908 above 25% w/w demonstrated sol-gel transition at body temperature, shear-thinning properties for easy injection, and physical stability[2]. The incorporation of polymeric nanoparticles (NPs) within the copolymeric matrix can affect the viscoelastic properties and the syringeability of P908 hydrogels. In particular, their composition and concentration are able to modulate the rheological profiles of hydrogels. We demonstrated that various NPs can be embedded within P908-based hydrogels obtaining novel multifunctional formulations and innovative depot systems to be used for several pharmaceutical applications (nanovaccination, wound healing, antitumor, and anti-inflammatory therapy).

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OC7

Geopolymeric Films based on halloysite clay nanotubes for environmental applications

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The development of smart materials with customized properties for environmental applications presents a significant challenge for scientific and technological research. Halloysite (HNTs) is a natural nanoclay characterized by its unique hollow tubular structure and distinct surface chemistry. First, we developed hybrid films made from halloysite nanotubes and cellulose sourced from Posidonia oceanica sea balls (egagropili)[1], a marine waste that accumulates along Mediterranean beaches. Despite the high content of clay nanotubes, the composite films displayed macroscopic properties similar to pure cellulose. The addition of halloysite improved the thermal stability of cellulose but led to a decrease in tensile strength. However, the cellulose/HNT composite films still demonstrated competitive performance in terms of elasticity and mechanical resistance. These films were further converted into geopolymers, resulting in a significant increase in rigidity and stress at break, particularly in composites with the highest HNT content (80 wt%). They represented an initial step toward developing composite materials by valorising egagropili and geopolymers in construction field. After this first stage, self-standing inorganic films with varying thicknesses (ranging from 60 to 300 μm) were fabricated through the entanglement of long Patch halloysite clay nanotubes (PT_Hal), which form interconnected fibrous structures thanks to the outstanding length of their tubes. The self-assembly of very long natural clay nanotubes offers a powerful approach for creating thermo-stable inorganic thin films suitable for environmental applications[2]. The film thickness played a crucial role in providing specific properties such as transparency, mechanical strength, and water absorption. All PT_Hal-based films are fire-resistant and thermally stable, preventing flame propagation. Even after direct exposure to flame, the films show no signs of deterioration or visible alterations. PT_Hal films were also used as precursors for developing functional materials through alkaline activation treatment, which produce highly porous geopolymers. Thanks to this property, the geopolymer shows potential for CO_2 capture, doubling the CO_2 adsorption efficiency compared to the original inorganic film, emphasizing its potential as an effective sorbent.

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OC8

In silico design and synthesis of new potential antibacterial drugs and ligand-protein interaction studies for new active molecules against COX-1 receptor.

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The design of new drugs is a fundamental aspect of the pharmaceutical industry. Expanding the therapeutic spectrum of existing bioactive molecules and developing new therapies are the primary objectives of pharmaceutical research. In recent years, the study of COX-1 has gained significant attention, especially with the discovery of its overexpression in certain human pathologies[1]. The design of new compounds, derived from existing ones, can be challenging and time-consuming. Regardless of the protein target, it is often difficult to determine which modifications will improve the ligand-protein interactions. These challenges result in a considerable waste of time and resources in chemical laboratories. Molecular Docking could be the solution, because it is an effective and competent tool for in silico screening that permits to evaluate at the same time a lot of compounds. Starting from a rich online database of easily available and bioactive compounds[2], we searched for some molecules that are like four compounds templates, which are potent COX-1 inhibitors from the ***diarylheterocycle*** class, known for their notable biological and antibacterial activities[3]. These compounds were then imported into the FLAP software. Software FLAP identifies interaction fields (MIFs), computed in GRID[4], and operates in a structure-based virtual screening (SBVS) mode, studying interactions between the molecules being analysed and the calculated protein pockets[4]. These virtual screening, with the support of literature searches, can be excellent starting points for the construction of a large database of compounds. Additionally, a parallel line of research concerning green pistachios has enriched this project by providing a diverse source of bioactive compounds. According to the literature, many of these molecules show promise as starting points for the development of new antibiotics, antibacterials, and anti-inflammatory drugs[5]. To this end, an initial extraction technique for the polyphenolic components[6] was developed, aiming to capture a comprehensive profile of these molecules to further enrich the database. The novelty of this project lies in the application of in silico methods to reveal both the physicochemical characteristics and ADME (Absorption, Distribution, Metabolism, and Elimination) properties of these compounds, thereby facilitating the design, synthesis, and/or extraction of new antibacterial and anti-inflammatory drugs, including potential COX-1 inhibitors.

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OC9

Structure-based drug design and virtual ligand screening for the discovery of GPER targeting compounds

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The G protein-coupled estrogen receptor (GPER) is involved in the complex effects of estrogens in diverse pathophysiological conditions including neurodegenerative diseases, immune system dysfunctions, metabolic and cardiovascular disorders. Moreover, it has been shown that GPER may play a role in the progression of several types of cancer. Therefore, GPER holds potential as a promising therapeutic target for the development of novel anticancer drugs.

Although the complete crystallographic structure of GPER has not yet been resolved, integrated approaches, such as structure-based drug design, virtual ligand screening and the generation of accurate molecular models, have enabled the identification of selective ligands, shedding light on its mechanism of action and biological functions. In line with these efforts, we performed molecular docking studies on a 3D structural model of the receptor in order to explore the ability of various compounds to act as selective ligands[1].

Herein we focused our attention on palbociclib, a known cyclin D1-cyclin dependent kinases (CDK) 4/6 inhibitor. When combined with hormone therapy, this compound has demonstrated noteworthy efficacy during the treatment of estrogen receptor (ER)-positive and HER2-negative advanced breast cancer (BC) [2]. Despite these achievements, the frequent emergence of palbociclib resistance, that seems to be related with GPER activity, represents a major clinical challenge. To further elucidate the mechanism responsible for the resistance, molecular docking simulations were conducted on a model of the protein. The binding mode of palbociclib with the receptor was compared to that of two GPER agonists, G-1 and E2. As a result, palbociclib exhibited a behaviour similar to that of both the known ligands, interacting with key residues within GPER binding site. Overall, our findings underscore the potential of palbocilcib as a selective ligand supporting the results of previous biological studies. Furthermore, these results provide new insights into the molecular events associated with the resistance to palbociclib in BC highlighting the crucial role of GPER in mediating the estrogen effects.

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OC10

Discovery and structure-based optimization of potent sigma receptors ligands

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Sigma receptors (SR) are among the most intriguing biological targets for the discovery of innovative drugs across a wide range of pathologies. Notably, the S1R subtype is highly expressed in both the central and peripheral nervous systems, particularly in regions crucial for neuroprotection, neuroinflammation, neurotransmission, and neuroplasticity. Dysregulation of S1R has been linked to various neurodegenerative diseases, pain syndromes, stroke, and retinal degeneration.[1] Over the years, piperidine and piperazine derivatives, as well as spirocyclic and diazabicyclo compounds, have garnered significant interest in the development of bioactive compounds.[2] The incorporation of these moieties into a molecule – taking into account the variable *N–N* distance dictated by specific structures – provides a unique spatial arrangement that can significantly influence key parameters such as potency, selectivity, and physicochemical properties.

In recent years, our research group has been focused on developing several new classes of small molecules with high affinity for SR. Our iterative optimization process follows a structure-affinity relationship approach, which includes: (i) designing new candidate ligands, (ii) conducting *in vitro* radioligand binding assays, (iii) iteratively refining compounds based on their affinity and selectivity, (iv) identifying potential protein-ligand interactions through computational studies, and (v) synthesizing new compounds for further pharmacological evaluation. The most promising compounds have undergone *in vitro* toxicity assessment and *in vivo* evaluation of their functional profiles. Progresses towards the identification of lead compounds as S1R ligands will be fully disclosed.

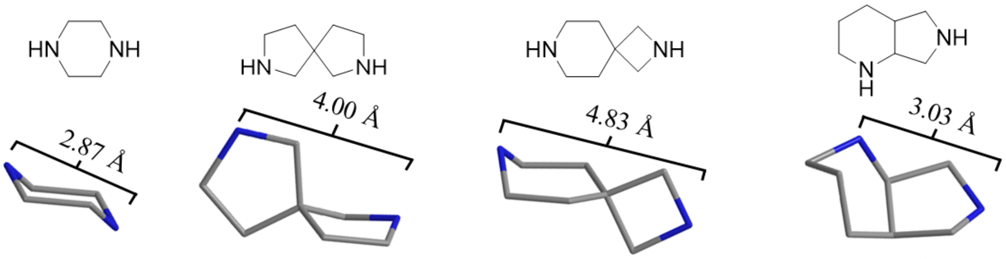

Figure 1. Diverse moiety integration for the development of novel SR ligands.

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OC11

Innovative Approaches in Oncology: Insights from Density Functional Theory on PACT Mechanisms

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Metal-based therapies were fundamental in the treatment of cancer over the past four decades, primarily due to the identification of the antiproliferative properties of cisplatin, which continues to be one of the most widely used chemotherapeutic agents in the world. With the aim to overcome the well-known limitations associated with the actual cancer treatments and increase the range of treatable cancers, novel alternative therapeutic strategies have been proposed in recent years. In this respect, photoactivated chemotherapy (PACT) is an emerging and fascinating light-assisted treatment of cancer.

The mechanism of action of PACT anticancer prodrugs involves chemical changes upon light irradiation generating active drugs in the excited state that can act with novel or poorly understood mechanisms of action. Currently, several types of coordination compounds containing Pt(IV), Re(I), and Ir(III) together with Rh(III) and Ru(II) are under investigation for their application in PACT.[1-6]

The search for optimal photoactivated chemotherapeutic agents is currently ongoing, and computational studies provide valuable information to elucidate photodecomposition pathways and monitor chemical reactions of light-induced excited states. Therefore, the rationalization of existing compounds and the design of new molecules with markedly enhanced antitumor activity is enabled allowing the advancement in the field of photoactivated chemotherapy. Here, we present the outcomes of a comprehensive density functional theory (DFT) investigation, utilizing a novel computational workflow tailored for studying the photoinduced activation mechanisms in PACT therapy. The outcomes of the exploration of the photophysical properties of recently synthesized metal-based complexes are reported and a detailed elucidation of the photodissociation mechanism is provided.

OC12

Vibrationally-resolved deep-red circularly polarized luminescence spectra of C70 derivative through gaussian curvature analyses of ground and excited states

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Over the last years, the interaction of fullerene with circularly polarized light has attracted growing attention for potential electronic and optical applications[1]. However, in literature there is only one example of fullerene derivative capable of emitting circularly polarized light, showing an active circularly polarized luminescence (CPL) signal in the deep-red visible region[2]. This unique luminophore offered us the possibility to study the connection between the topological features of C70 spheroid and its chiral emission properties. In light of these considerations, we proposed a theoretical protocol that combines three different steps: 1) The Ball Pivoting Algorithm for C70 surface reconstruction. 2) The discrete gaussian curvature analysis in the ground (S0) and excited states (S1). 3) The computation of the vibrationally-resolved CPL spectrum. The first step allowed us to extract useful information that linked the topological shape of C70 to the sp^2 carbon network chemistry. The DFT benchmark in the second step guided us in grasping the best functional for the C70 curvature simulation in the ground state, spotlighting how B97D3 excellently succeed for this task. The curvature investigation in the first excited state showed that (for all the twenty exchange-correlation functional tested) the C70 fragment is more curved in S1 than in S0. The final step collected the topological information from the previous sections to provide a detailed overview of the theoretical factors (such as the quantum formalism, the potential energy surface description and the transition dipole moment approximation) impacting on the C70 vibrationally resolved CPL spectrum. We found that the adiabatic hessian model coupled with the Franck-Condon Herzberg-Teller approximation computed at PW6B95D3/6-311G(d,p) level provides excellent results in emulating the band-shape and position of the experimental CPL spectrum.

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OC13

Photo-thermocatalytic CO_2 methanation on SiC/hydrotalcites-derived catalysts

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The development of new catalysts capable of activating hybrid photo-thermocatalytic processes allows to implement significantly the catalytic performance compared to simple photo- or thermocatalytic processes.[1] The aim of this work was to synthesize a set of photo-thermocatalysts based on the interaction between SiC and mixed oxides derived from hydrotalcites. The hydrotalcites-derived materials present excellent thermocatalytic properties which are implemented thanks to the photo-thermal properties of SiC.[1] Two different hydrotalcites (containing Mg or Zn, Co and Al ions) were synthesized by hydrothermal method; the corresponding mixed oxides were obtained by calcination, promoting the formation of photocatalytic active species such as ZnO and $ZnAl_2O_4$. Finally, by addition of SiC (in a ratio of 1:1), the two photo-thermocatalysts were obtained: IDT Mg-Al-Co+SiC and IDT Zn-Al-Co+SiC. These samples were then tested in the CO_2 methanation process, for which a maximum selectivity value of 71% towards CH_4 was obtained in photo-thermocatalytic approach, operating at 250°C. This represents a significant improvement over the thermocatalytic process for which the maximum selectivity obtained towards CH_4 is 36%, working at 350°C. The addition of SiC improved the photo-thermocatalytic performance: it has favored the widening of the optical band-gap increasing the range of wavelengths that the material is able to absorb; has modified the basic sites of the hydrotalcite-derived catalysts promoting CO_2 adsorption and activation; has activated the photo-driven mechanism by converting the light into self-generated heat.[2]

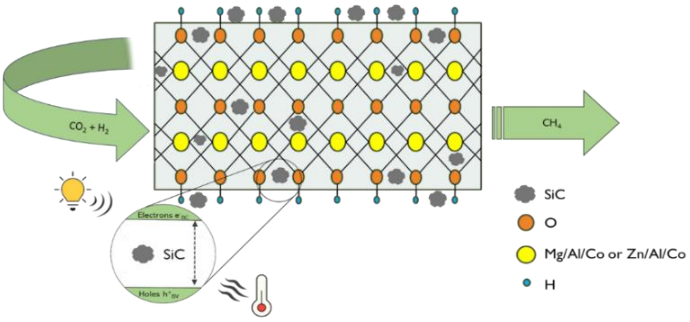

Figure 1. Graphical abstract of the CO_2 methanation process using the photo-thermocatalysts

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OC14

Designing of a Monolithic Photo-Fenton Catalyst from a Fungal Hydroxypyrone Derivative

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In response to the demand for eco-sustainable materials,[1] we developed an innovative catalyst derived from kojic acid, a natural *Aspergillus* metabolite.[2] Functionalized with an acrylic group, the resulting porous organic polymer (C-HPO) (Figure 1, a) efficiently chelates heavy metals like mercury, copper, and iron, demonstrating its potential for environmental remediation. Coordinating iron ions with C-HPO created a photo-Fenton-like system (C-HPO/Fe), effectively degrading emerging contaminants like lomefloxacin, doxycycline, desethyl atrazine, and methylene blue. Remarkably, just 2 mg of the C-HPO/Fe achieved near-complete pollutant degradation, underscoring its promise for sustainable environmental cleanup and catalysis.

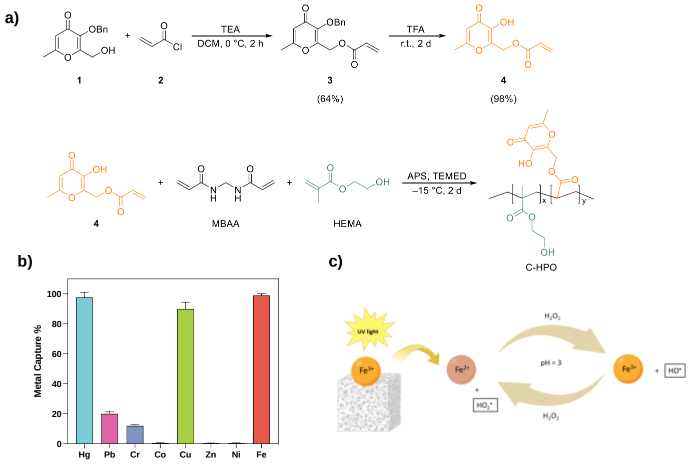

Figure 1. **a)** Synthetic route of C-HPO catalyst; **b)** Percentage of metal ions captured by C-HPO; **c)** Schematic illustration of photo-Fenton-like mechanism.

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OC15

Ammonia synthesis via plasma-assisted electrochemical nitrogen conversion at ambient conditions

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Ammonia (NH_3) is an essential component of the chemical industry, primarily used in the production of fertilizers, pharmaceuticals, and explosives. However, the traditional Haber-Bosch process, while effective, is highly resource-intensive, requiring significant energy and capital investment and contributing substantially to greenhouse gas emissions.[1] Electro-, photo-, and plasma catalysis are promising advancements in catalytic technology, offering sustainable alternatives for traditional industrial processes.[2] In this study, we present a novel aqueous electrochemical device incorporating a micro-plasma cathode for the direct synthesis of ammonia under ambient conditions. Ammonia production is achieved through solvated electrons generated by the interaction of the plasma jet with the aqueous solution, acting as powerful reducing agents without the need for additional reagents or catalysts. This approach overcomes the limitations of traditional catalytic systems in terms of both activity and long-term catalyst stability. We report, for the first time, the optimization of this plasma-electrochemical device by adjusting key operational parameters such as the plasma-liquid surface gap, flow rate, cell potential, and current, resulting in enhanced Faradaic Efficiency (FE%) and production rate. Preliminary experiments indicate a FE% exceeding 50% for NH_3 after 30 minutes of reaction, with a production rate of approximately 0.17 mg h^{-1}. Although further investigation into other setup parameters is necessary, the initial results demonstrate the potential of this approach as a sustainable method for nitrogen fixation.

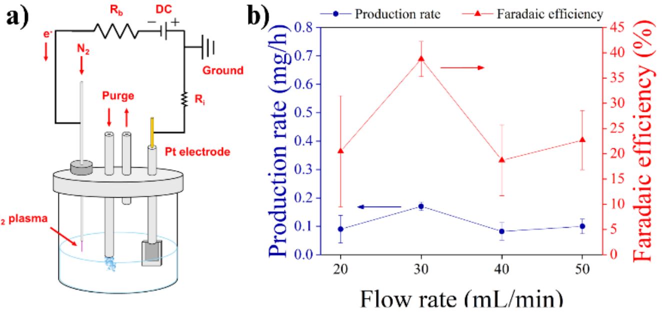

Figure 1. a) Plasma-electrochemical cell and b) ammonia production rate (mg h^{-1}) with corresponding FE%.

Acknowledgements*: This work is funded by the EU through the SUPERVAL (ID: 101115456) H2020 Project, and by the MUR through the PRIN Project HYDREAM (2022YXHXH5ID), which are gratefully acknowledged.*

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OC16

Composite photocatalysts prepared with materials from spent Li-ion batteries and g-C_3N_4 for the photoreforming of organics in aqueous solution to obtain H_2

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Every year, millions of tons of spent lithium-ion batteries (s-LIBs) are generated. The recycling methods to recover the precious metals they contain, mainly Ni, Co and Li, are energy-intensive, non-selective and expensive. The development of processes for the direct reuse of s-LIBs is an urgent issue[1]. The current work is an attempt to develop innovative materials, as graphitic carbon nitride (g-C_3N_4) enriched with a metal-based co-catalyst obtained from the mechanical grinding of the mixture of anode and cathode powders contained into the spent s-LIBs, called *black mass* (BM).
The photoreforming technology of aqueous solutions of organics is aimed at addressing energy and environmental concerns by obtaining H_2 from water and simultaneously oxidizing organic molecules to other higher added-value substances. In the last decade, carbonaceous materials such as C_3N_4 have demonstrated good performances as free metal photocatalysts in this type of reactions. Graphitic carbon nitride (g-C_3N_4) is a semiconductor that possesses optimal characteristics to be used as a photocatalyst even under solar irradiation, however it can suffer from recombination of the photogenerated electron-hole pairs with consequent decrease in photocatalytic activity. Its coupling with various materials can improve its performance. In fact, g-C_3N_4 composites with graphene[3] or TiO_2[4] have given excellent results in terms of H_2 productivity by photoreforming.
In this research, BM from s-LIB, containing ca. 60 % w/w of Co, was used either raw or after being oxidized or reduced with H_2 at 600 °C for 6 h. g-C_3N_4 was prepared by calcination of melamine, urea or thiourea. Various sets of composites were prepared by following some different strategies to obtain g-C_3N_4/BM photocatalysts with an amount of BM enough to bring to the composite a content of Co in the range 0.5 to 2 % w/w. Additionally, hydrochar (HC) obtained from the hydrothermal combustion of orange peel waste was also used as a co-catalyst. The obtained materials were tested for H_2 production using aqueous solutions of ethanol, glycerol or triethanolamine irradiated with UV or natural solar light. Photoreactivity was performed in the absence or presence of 1% Pt. The best results were obtained with catalysts containing g-C_3N_4 with a 1% of Co from BM. The solid obtained by grinding g-C_3N_4 and BM in a planetary mill gave a H_2 productivity of 0.9 mmol h^{-1} g^{-1} whereas the composite obtained by grinding melamine and BM, followed by calcination at 520 °C for 2 h gave 1.7 mmol h^{-1} g^{-1}. The best material was obtained by ball-milling melamine and the BM obtained after successive cycles of reduction and oxidation giving a H_2 productivity of 2.2 mmol h^{-1} g^{-1}.

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OC17

The usefulness of the cryogenic zone compression gas chromatography-mass spectrometry approach for analysis of polycyclic aromatic hydrocarbons in food

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This study focuses on developing a simple method for the semi-quantitative determination of 16 polycyclic aromatic hydrocarbons (PAHs) in extra virgin olive oil (EVOO) using cryogenic zone compression (CZC) gas chromatography coupled with single quadrupole mass spectrometry (GC-QMS). By employing CZC through a loop-type cryogenic modulator to enhance signal-to-noise ratios (*s/n*), the sample preparation process was simplified, requiring only a single extraction with 500 µL of acetonitrile prior to injection. The CZC GC-QMS method, which adheres to the principles of green analytical chemistry, demonstrated a 14-fold average increase in *s/n* compared to conventional GC-QMS.

The method's limits of quantification ranged from 0.07 to 8.33 µg kg^{-1}. Accuracy, measured at 2 and 10 µg kg^{-1} concentrations, ranged from 82% to 103%. Intra-day and inter-day precision at these concentration levels ranged from 1.9% to 14.7% and 5.9% to 9.1%, respectively, with recovery values at 10 µg/kg ranging from 24% to 99%. A positive matrix effect was observed for all PAHs analyzed. Two PAHs were detected (in selected ion monitoring mode) in six of the ten EVOO samples tested, with no more than one PAH found per sample.

OC18

An integrable sensoristic platform for β-amyloid based on supramolecular interactions

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An early-stage diagnosis could significantly improve the prognosis of severe diseases such as Alzheimer's (AD). The key is to find alternative platforms for the improvement of clinical diagnostic methods. In this scenario, nanotechnology gains the possibility to tailor materials and devices on purpose. Following this lead, we prepared and characterized, using dynamic light scattering (DLS), cyclic voltammetry (CV) and scanning electron microscopy (SEM) techniques, a sensitive nanohybrid integrable in electrochemical detection platforms for the recognition of Aβ-40 and Aβ-42 β-amyloid peptides, selected as biomarkers of AD. Using the thin film hydration method, we decorated the surface of graphene oxide (GO) with the amphiphilic cyclodextrin heptakis[6-deoxy-6-hexadecylthio-2-poly(ethyleneglycol)]-β-cyclodextrin (SC16OH) nanovesicles entangling the hydrophobic peptide conjugate Ferrocene-$(PEG)_4$-KLVFF (Lys-Leu-Val-Phe-Phe, Aβ (16–20)) or (Fc-Pep), selected as the recognition entity of Aβ-40 and Aβ-42 [1]. The supramolecular assembly, with or without GO, was prepared in view of the next integration in an electrochemical sensing platform towards β-amyloid detection.

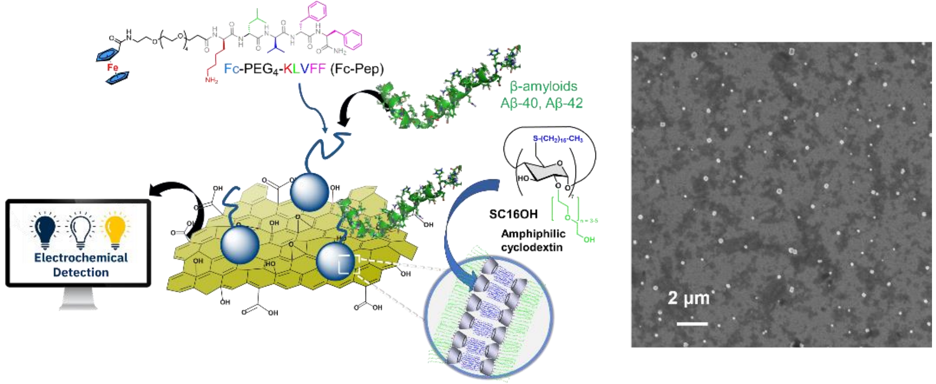

Figure 1. Graphical abstract.

Acknowledgements

This project is supported by the PNRR project SAMOTHRACE "SiciliAn MicrOnanoTecH Research And innovation CEnter" ECS 00000022 - CUP B63C22000620005

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OC19

Macroporous Porphyrin Cryogels: High-Efficiency Mercury Adsorption and Colorimetric Sensing

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New porphyrin-based cryogels were synthesized by incorporating porphyrin units into a macroporous polymeric structure. These materials combine the macroporosity, versatility, and structural robustness of cryogels with the unique properties of the porphyrin ring, such as the ability to capture pollutants and change color in the presence of metals.[1,2] The cryogels were developed to simultaneously remove and detect metal ions, such as mercury (Hg^{2+}). Aminoethyl methacrylate (AEMA), functionalized with meso-tris(N-methyl-4-pyridyl) mono(4-carboxyphenyl) porphine trichloride (PORPH), was cryo-polymerized with acrylic monomers in varying ratios from 2% to 20% w/w. The materials were tested for Hg^{2+} adsorption, showing a visible color change in the presence of mercury. The hydroxyethyl methacrylate-based cryogel containing 20% porphyrin achieved a maximum adsorption capacity (Qe) of 56.4 mg/g at neutral pH. To improve the adsorption properties, a methacrylic acid-based cryogel containing 2% porphyrin was synthesized and subsequently functionalized with thiol groups (-SH), resulting in an increased mercury (Hg^{2+}) adsorption capacity of 720 mg/g. Moreover, the color shift from red to green upon mercury adsorption opens new perspectives for developing multifunctional devices capable of simultaneously detecting and removing metal pollutants.

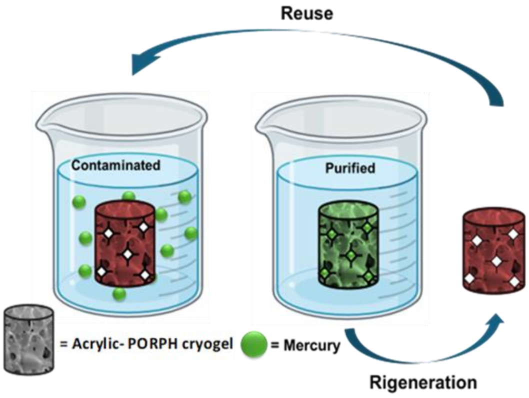

Figure 1. Schematic illustration of the monolithic cryogel incorporating porphyrin and its color changing in response to mercury adsorption.

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OC20

Turning local waste into resource: *Opuntia ficus-indica* cladodes and *Prunus dulcis* husk as adsorbents of lead ions

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Water pollution by toxic metal ions is a matter of great concern and poses a serious threat for humans and all living organisms. For this reason, a large part of the scientific community is focused on finding a suitable removal strategy that is also in line with the principles of environmental sustainability and circular economy[1]. As an alternative to conventional chemical treatments, adsorption is considered one of the most attracting removal techniques, in particular when the employed adsorbents come from waste platforms[2]. In this contribution are presented the results achieved using *Opuntia ficus-indica* cladodes (**OFI**) and *Prunus dulcis* husk (**PD**) as adsorbents for lead ions from aqueous solutions. Batch adsorption experiments were carried out with both OFI and PD in aqueous solutions at pH = 5, t = 298 K and $I \rightarrow 0$ mol $L^{-1}$and in the ionic media $NaNO_3$ and NaCl 0.1 mol L^{-1}. The effect of pH and of chloride ions concentration on the adsorption ability of the biomasses were also evaluated carrying out adsorption experiments at pH = 2.0, 3.0, 5.0 and 6.0 and in a wide NaCl concentration range ($0.1 < I$ (mol L^{-1}) < 0.5). The kinetic of lead ions adsorption onto both biomasses was studied in $NaNO_3$ 0.1 mol L^{-1} at pH = 5, in the temperature range 288 – 308 K. Both adsorbents were previously characterized by ATR-FTIR analysis and pH_{pzc} measurements. The lead ions adsorption onto biomasses was well described by Langmuir isotherm equation. The OFI biomass showed the highest q_m value. The ionic medium reduced the adsorption capacities of OFI and PD, in particular NaCl whose anion forms Pb^{2+} complexes reducing the concentration of the free metal ions. OFI adsorption ability was less effected by pH variations compared to PD. The kinetic of adsorption was well described by pseudo-second order equation. Adsorption-desorption experiments in column evidenced a satisfy recyclability of both biomasses when HCl 0.1 mol L^{-1} was used as extracting solution. Finally, OFI, as the best adsorbent, was also tested in a continuous-flow fixed-bed column carrying out breakthrough curves.

Acknowledgements

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OC21

Nanoformulations of cosmetic interest for the cutaneous uptake of nickel

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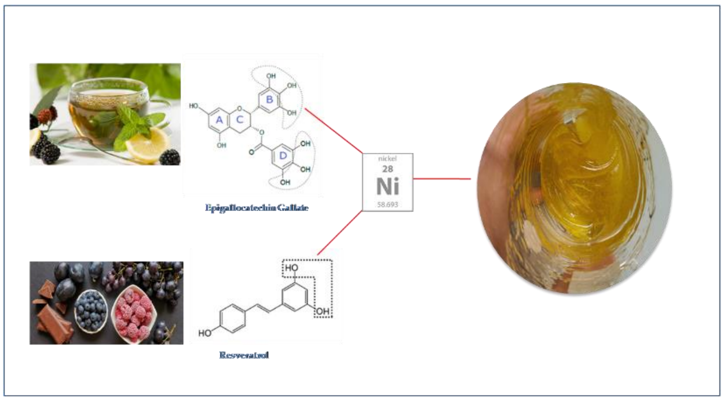
Cosmetic products contain numerous metals used as pigments, UV filters, preservatives, antiperspirants and antimicrobial agents, which are responsible for allergic skin reactions, the most common being nickel[1]. To reduce skin penetration of Ni, innovative pharmaceutical formulations such as lipogels with chelating action against the metal ions themselves can be used[2]. Chelation therapy allows a chelating agent to combine with metal ions to form a stable ring structure called a chelate. The chelate structure is more soluble in water than the toxic metal, which facilitates removal of the toxic metal from the tissue and its excretion by the kidneys. The aim of the following work was to evaluate the chelating properties against nickel ions of different types of lipogels containing flavonoids such as resveratrol and epigallocatechin gallate with chelating activities largely dependent on the number and position of their hydroxyl groups.



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OC22

Expanding SUPRADES beyond cyclodextrins: preparation and study of resorcin[4]arene/choline chloride binary system[§]

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A preliminary thermal and spectroscopic investigation of different resorcin[4]arene-like macrocycles and choline chloride as possible components of binary eutectic solvent systems is presented herein. NMR relaxometry measurements, performed by the Carr-Purcell-Meiboom-Gill (CPMG) sequence based on spin- echo decay,[1,2] were used to study such systems at a molecular level. Results were elaborated by ILT (Inverse Laplace Transform), as the NMR-ILT echo decay signal analysis provides the T_2 relaxation time, which can be ultimately correlated with the interaction between the two components toward the formation of a supramolecular structure.[1,2] The performed chemical-physical characterization indicated the possibility that the investigated macrocycle/choline binary system could represent novel SUPRADES system, albeit not based on cyclodextrins.

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OC23

Development of Peptide-Based SARS CoV-2 M^{pro}/hCatL Dual Inhibitors as Antiviral Agents

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SARS-CoV-2 is the virus responsible for COVID-19. Despite the significant efforts of the scientific community, the long-term efficacy of antibodies and the emergence of new variants remain uncertain for the coming years. In light of this, the development of effective antiviral agents continues to be a priority in the fight against COVID-19. Main protease (M^{pro}) is a crucial cysteine protease of SARS-CoV-2 involved in the cleavage of polyproteins into non-structural proteins.[1] In addition to the viral components, human cathepsin L (hCatL) plays a key role in facilitating the virus entry into host cells.[2] Starting from hit-compound **1**,[3] a series of peptide-based Michael acceptors as potential dual M^{pro}/hCatL inhibitors was developed (Figure 1). The new molecules contain a methyl vinyl ketone warhead, a cyclic pentatomic glutamine surrogate at the P1 site, a panel of aliphatic amino acids at the P2 site, and a monofluoro-substituted benzoyl group as the *N*-terminal cap. Seven M^{pro}/hCatL dual inhibitors with K_i values in the micromolar and nanomolar range against the viral and human targets, respectively, were identified. Three of them showed promising EC_{50} values in the low micromolar range against Huh-7-ACE2 infected cells without cytotoxicity. Selectivity for the targets was assessed. Docking studies were conducted to gain comprehensive insight into the structure-activity relationship.

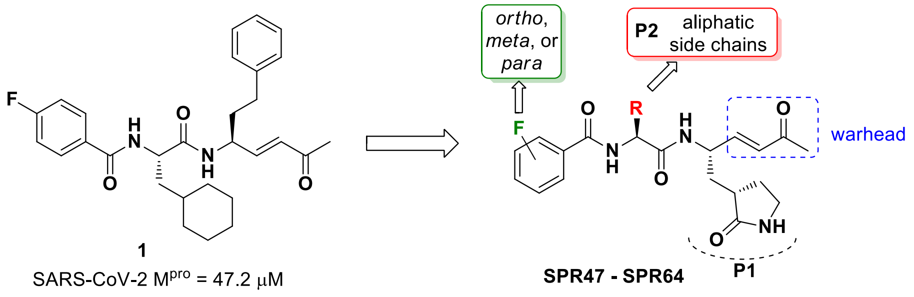

Figure 1. Design of novel dual inhibitors **SPR47-SPR64**.

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OC24

Thiazole-based compounds as promising fusion inhibitors of influenza A/H1N1 virus

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Influenza A virus (IAV) is a highly contagious respiratory pathogen responsible of seasonal and pandemic flu. Despite the development of several vaccines and antiviral drugs, the rapid emergence of drug resistance points out the need for new therapeutic approaches.[1]

The hemagglutinin (HA) protein represents a key drug target in the inhibition of the IAV entry process, playing an essential role in the initial phases of influenza A infections.[2] Since thiazoles have been widely investigated for their antiviral properties,[3,4] a library of thirty *N*-(2-phenyl-1,3-thiazol-5-yl)benzamides of type **1** has been synthesized and evaluated against different influenza viruses (A/H1N1, A/H3N2, B).

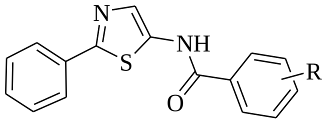

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Figure 1. Chemical structure of *N*-(2-phenyl-1,3-thiazol-5-yl)benzamides.

In vitro assays revealed promising derivatives potently inhibiting the IAV A/H1N1 replication in MDCK cells with EC_{50} values in the low micromolar range for different A/H1N1 strains. The A/H1N1 pseudovirus entry assay was also performed to investigate their mechanism of action, confirming a strong inhibition of the HA-mediated entry process.

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OC25

Asymmetric Salphen Complexes and Selective Targeting of G-Quadruplex Structures

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Over the past decade, significant progress has been made in developing DNA-targeting drugs, particularly those that selectively bind non-canonical DNA structures like G-Quadruplexes (G4s), which form from G-rich sequences in DNA and RNA. These four-stranded structures, composed of stacked guanine tetrads, are in conserved regions of human and viral genomes, making them promising targets for anticancer and antiviral therapies.[1] Metal complexes of Schiff base ligands show potential for selective G4 binding due to their chemical and structural properties.[2]

In our study, we synthesized novel asymmetric Salphen metal complexes with neutral and charged substituents (Figure 1) and evaluated their selectivity for viral and human G4 structures using spectroscopic and computational methods. Preliminary results indicate that Ni(II)-based complexes have strong selectivity for G4 motifs. Biological studies further demonstrate improved cellular internalization of these complexes compared to neutral and doubly charged counterparts. We are also developing a machine learning model to predict the activity of new Salphen complexes, offering a valuable tool for future drug development.

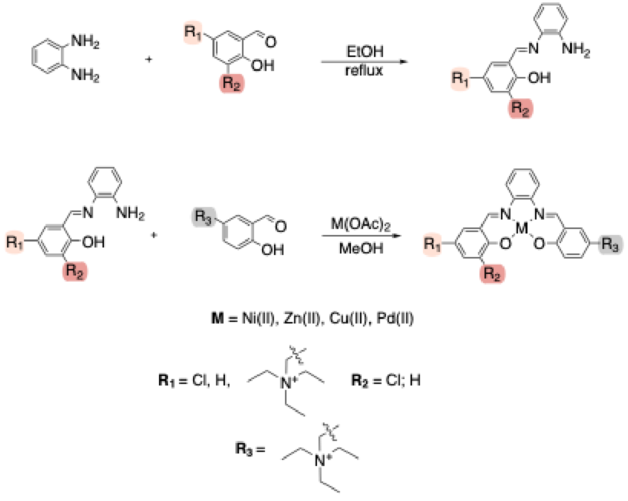

Figure 1. Scheme reaction of the new Salphen metal complexes

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OC26

Development of Drug Delivery Systems based on MagnetoCyclodextrins for osteosarcoma treatment

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Superparamagnetic iron oxide nanoparticles (SPIONs) are valuable tools for cancer diagnosis and therapy due to their unique characteristics, including nanoscale size, specific surface functionalization, and responsiveness to external magnetic fields. These properties make them the ideal candidates for theranostic applications[1]. While some SPIONs are commercially available as imaging contrast agents, only two have been approved for cancer treatment, and none have yet been utilized specifically for osteosarcoma therapy.

We investigated the use of cyclodextrins (CD) as a capping agent of oleic acid-stabilized SPIONs (OA-SPIONs) to develop biocompatible and biologically stable MagnetoCyclodextrins for osteosarcoma treatment. Thirteen types of CDs, including α, β, and γ- CD and their polymeric derivatives, were investigated. From our studies emerged that six types of CDs were able to entrap oleic acid chains, resulting in stable water soluble MagnetoCyclodextrins. Among them, Sugammadex (SGX, BRIDION®), a FDA and EMA-approved γ-CD used as neuromuscular blocking agents antidote[2-3], was deeply investigated. Notable, MagnetoSugammadex (MNP-SGX) demonstrated reproducibility as a monodispersed, biocompatible nanoplatform, maintaining stability in water, PBS, cell culture media, and blood plasma for at least 24 h.

Acknowledgments

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OC27

Design, Synthesis, and Biological Evaluation of New Ligands as Potential Therapeutic Agents for Persistent Pain Treatment

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The use of multitarget opioid drugs, alongside σ1R antagonists, represents a promising strategy for the treatment of various painful conditions. Among these, the *N*-normetazocine scaffold has garnered significant attention in medicinal chemistry as a foundation for novel therapeutic agents. Notably, the *N*-normetazocine-based compounds (–)-LP1 and (–)-LP2, which exhibit a dual-target profile toward MOR and DOR, have shown considerable efficacy in preclinical inflammatory and neuropathic pain models. SAR studies have been instrumental in identifying the chemical groups responsible for these biological effects, leading to the development of novel LP1 and LP2 analogs that demonstrated potent, dose-dependent analgesic effects *in vivo* (Figure 1).[1] Further investigation into the stereochemistry of *N*-normetazocine revealed the σ1R selective antagonist (+)-(2*R*/*S*)-LP2, which significantly attenuated the second phase of the formalin test and effectively inhibited mechanical allodynia in chronic constriction injury rats.[2] Additionally, natural compounds have emerged as valuable starting materials for synthesizing diverse σ1R ligands. Enantiomerically pure morphans, derived through chiral pool synthesis, showed a selective affinity for σ1R. These findings highlight strategic chemical modifications that modulate receptor affinity, specifically targeting opioid and sigma receptors, key players in pain transmission pathways.

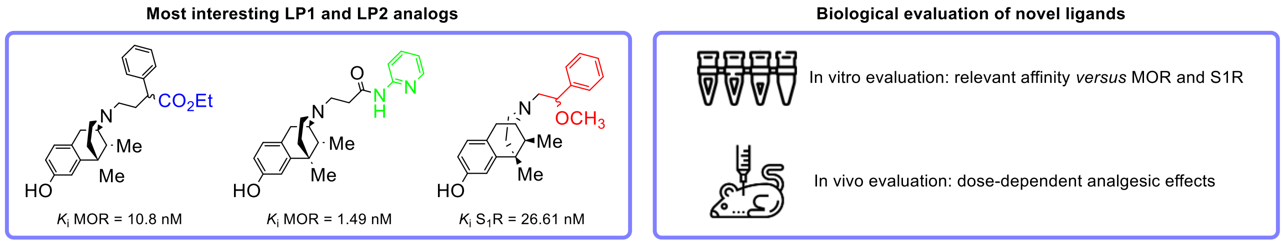

Figure 1. Some representative novel LP1 and LP2 analogs.

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OC28

“New Synthesis of 2-(Benzofuran-2-yl)acetamides”

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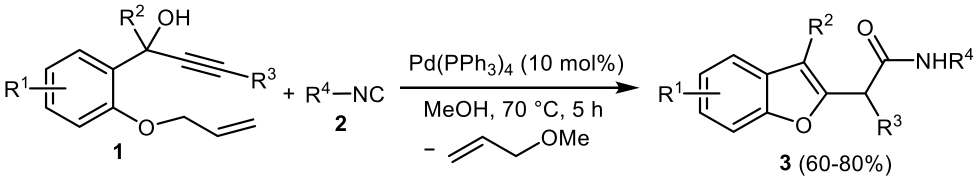
(2-(Benzofuran-2-yl)acetamides represent a class of organic compounds of particular interest, due to their significant pharmacological activities, including antifungal1 and anticonvulsant[2,3] activities, in particular. Their structural versatility makes them promising candidates for drug discovery and development, motivating research efforts aimed at developing new methods for their synthesis as well as at understanding their biological functions and therapeutic potential.
In this contribution, a novel catalytic method is presented, which allows the synthesis of 2-(benzofuran-2-yl)acetamides **3** starting from readily available 1-(2-(allyloxy)phenyl)-2-yn-1-ols **1** and isonitriles **2** and with $Pd(PPh_3)_4$ as simple catalyst (Scheme 1). Reactions are carried out in MeOH at 70 °C for 5 h.



Scheme 1

Formation of **3** derives from a mechanistic pathway involving an ordered sequence of steps, beginning with the oxidative addition of the phenoxyallyl moiety of **1** to Pd(0) followed by the insertion of **2** to give an (allyl)(imidoyl)palladium complex. The isonitrile group, being isoelectronic with CO, in a similar manner as carbon monoxide[4] is, in fact, able to insert into the palladium-carbon bond arising from the oxidative addition of a suitable substrate to Pd(0). Water attack to the (allyl)(imidoyl)palladium complex followed by β-H elimination from the H-O-C-Pd(allyl) moiety leads to formation of an allylpalladium hydride species (allyl)PdH and a 2-(3-hydroxybenzofuran-2(3*H*)-ylidene)acetamide intermediate. Reduction of the latter by (allyl)PdH and MeOH finally affords the desired (2-(benzofuran-2-yl)acetamides.

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OC29

H-bonding solvents influence on the conformation adopted by a novel calix[4]tube both in liquid and in solid phase

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A new octaurea-calix[4]tube (**UC4T**) has been obtained in three steps from the original Beer's *p-tert*-butylcalix[4]tube ionophore.[1] In a polar solvent (DMSO-d_6), **UC4T** rapidly interconverts between two identical conformations with C_{2v} symmetry for the two calix[4]arene subunits. However, in a less polar solvent mixture ($CDCl_3$/DMSO-d_6, 98:2), **UC4T** adopts an asymmetric structure. The complexation of cations inside the dioxyethylene ionophoric binding site of **UC4T** triggers a C_{2v} to C_{4v} symmetry rearrangement of the two calix[4]arene subunits, leading to the formation of a transient capsular dimeric species observed in solution. X-ray studies confirm **UC4T**'s ability to adopt different asymmetric conformations depending on its interactions with solvent molecules and two distinct crystal forms (α and β) of **UC4T** have been obtained. Notably, the pseudo-capsular 1D supramolecular polymeric arrays observed in the β form of **UC4T** assemble to create large parallel solvent channels.

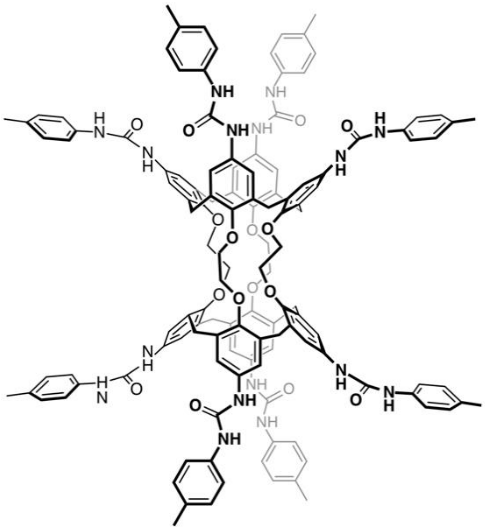

Figure 1. Structure of octaurea-calix[4]tube **UC4T**.

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OC30

UPCYCLING POLYCARBONATE WASTE: AN EFFICIENT ALTERNATIVE TO DISPOSAL

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Plastic waste is presently one of the most concerning issues, it is ubiquitous in the environment[1] and ecologically harmful. Precisely because of this, plastic recycling represents a possible way to overcome this issue. Furthermore, the recycling of plastic waste is an efficient alternative to waste disposal and it allows a closed loop-recycling which is the basis of the sustainable perspective.[2] In this framework, we investigated the recycling and the upcycling of polycarbonate (PC) under sonochemical conditions. The use of ultrasounds enables to carry out the reaction at room temperature. PC is used in DVDs, CDs toys, construction materials.[3] In particular, we studied the recycling of PC into bisphenol A (BPA) combining the use of task specific ionic liquids (TSILs) as catalysts, with ultrasounds. Furthermore, we also carried out the upcycling of polycarbonate to obtain ionic liquids (ILs). We performed the aminolysis of polycarbonate using N,N-dimethylethylenediamine and N,N-dimethylpropane-1,3-diamine as nucleophiles under ultrasound irradiation and, subsequently, we alkylated the ureas obtained with different alkyl halides in order to obtain ionic liquids.

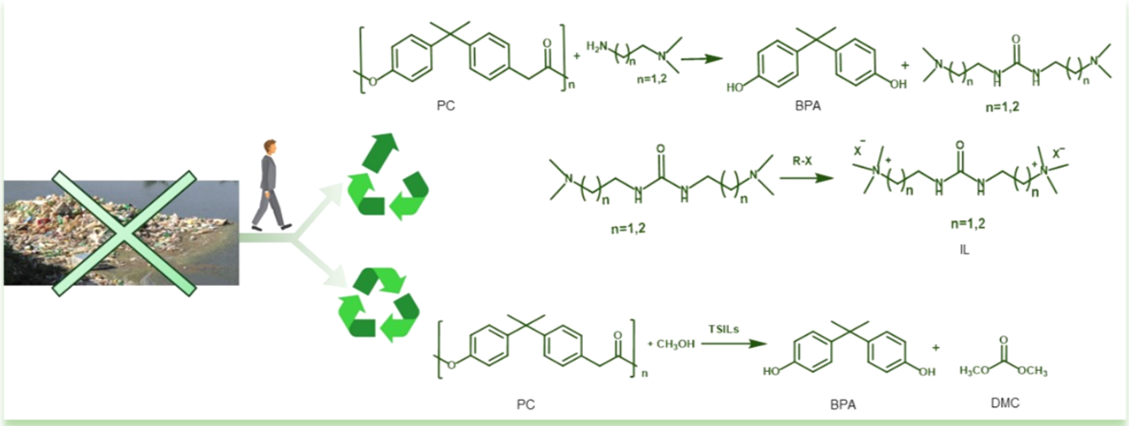

Figure 1. General reaction scheme

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OC31

Phenolic fraction and antioxidant activity of Palm oil

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Palm oil (PO) derives from the palm tree (*Elaeis guineensis*) fruit, and it is the most widely produced and consumed vegetable oil in the world.[1] Although it is strongly debated due to environmental and nutritional issues, there are a number of studies in literature that do not support some of these assumptions.[1,2]

Samples of POs from different West African and South American countries were subjected to the extraction of the phenolic fraction, achieved by using a methanol/water solution (80/20, v/v) as the extraction solvent. Total phenolic content (TPC) was evaluated by using *Folin-Ciocalteu* method, and the results are expressed as mg GAE (gallic acid equivalents)/100 g oil. Total flavonoid content (TFC) was expressed as mg QE (quercetin equivalents)/100 g oil. Antioxidant activity was determined by DPPH and ABTS radical assays. The phenolic profile was determined using an HPLC system, equipped with a Discovery C18 chromatographic column, coupled to an MSD API 4000 Q-Trap model mass spectrometer.

The values of TPC ranged from 17 to 75 mg GAE / 100 g. The values of TFC ranged from 6.5 to 55.4 mg QE / 100 g. The values of Trolox equivalent antioxidant capacity (TEAC) ranged from 403,3 to 1685,1 mg TEAC / 100 g in the case of DPPH, and from 1427,9 to 6859,4 mg TEAC / 100 g, in the case of ABTS. Ascorbic acid was used as the positive control in both assays.

Regarding the identification and quantification of individual phenolics, simple phenols, phenolic acids and flavonoids were identified and quantified in all samples. The most abundant were hydroxytyrosol, tyrosol, catechol, homovanillic acid, caffeic acid, pinoresinol, diosmetine, *o*-coumaric acid, and *m*-coumaric acid.

Interestingly, we have identified and quantified tyrosyl oleate (TyOle) and hydroxytyrosyl oleate (HtyOle) in PO for the first time. TyOle and HtyOle belong to lipophenols, an emerging subclass of phenolic compounds, characterized by the presence of a lipid moiety. In particular, TyOle and HtyOle represent significant forms in which tyrosol and hydroxytyrosol exist and display antioxidant, anti-inflammatory and anti-diabetic properties.[3-6]

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OC32

Differential proteomics approach to investigate human aging

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Aging is a multifactorial process involving physiological changes and an increased risk of chronic diseases. Therefore, it is essential to understand the molecular changes that occur during aging and to identify potential therapeutic targets for age-related diseases in order to improve overall health and lifespan.[1] Studies show that among the omics sciences, the proteomics is a promising approach to investigate and mitigate age-related cellular and molecular changes, particularly through the maintenance of proteostasis and protein quality control mechanisms.[2,3]

This research aims to perform differential proteomics analysis of red blood cells from individuals of different ages, to identify potential biomarkers in blood cells. The objective is to assess qualitatively and quantitatively the similarities and differences, at molecular level, among different age groups. Initially, the identification of biomarkers linked to age-related pathways or diseases was performed on *Mus musculus*, as an animal model. Blood samples were collected from young (6 months), middle-aged (12 months), and old (30 months) mice, from which whole blood cells were obtained. The membrane protein content was then extracted, separated and analyzed using an untargeted LC-MS/MS proteomics approach. MaxQuant software was used to process the raw data, and the resulting output files were subsequently analyzed using STRING to integrate all known and predicted associations between proteins that were either up- or down-regulated. Several of the identified differentially expressed proteins play a key role in physio-pathological processes, such as *Glycophorin-A* that is involved in the stability and shape of the erythrocyte membrane and is important for the function of Band 3 anion transport protein (SLC4A1). A similar approach will be applied to human blood samples to confirm the accuracy of the model. Overall, this study reveals some potential blood cell-protein biomarkers of aging and their possible correlation with immune system and metabolic pathways, providing another piece to unravel the complex puzzle of aging processes.

This work was financially supported by the Research Programm " Age-it- Ageing well in an ageing society", Spoke 2 - Project code PE0000015, CUP B83C22004800006, founded by the PNRR, Missione 4 "Istruzione e Ricerca".

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Comunicazioni flash

FC1

Development of nanomaterials based on halloysite as carrier for cIDPR molecules and PNA

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Development of multifunctional nanostructured systems is an appealing strategy to obtain nanomaterials with potential therapeutic applications.[1] Clay minerals, such as halloysite nanotubes (HNTs), represent appealing nanomaterial because of their high biocompatibility, low cost and the peculiar capability to cross cellular membrane, localizing themselves in the perinuclear area. Furthermore, the presence of an empty lumen, makes HNTs excellent systems for the loading and delivery of different biologically active species.[2] Peptide nucleic acids (PNAs) have emerged as promising agents for gene modulation. However, these molecules show a very low aqueous water solubility and poor cellular uptake that hamper their use.[3]

In this work, we propose a bifunctional nanomaterial based on covalently and supramolecular modified HNTs. Indeed, the HNTs outer surface was linked to PNA molecules capable of targeting the P1 promoter of the proto-oncogene bcl-2, whereas the empty lumen was loaded with different cIDPR molecules. The latter are cADPR mimetics, which function to regulate intracellular Ca^{2+} ions concentration.[4] The obtained nanomaterial was thorougly characterized by several techniques and its morphology was investigated as well. Finally, the nanomaterial was also tested in *vitro* to assess its potential for therapeutic use.

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FC2

A Comparative study of Two MIL-100(Fe) MOFs Synthesized via Conventional and Green Methods for Water Harvesting

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The increasing scarcity of water resources is one of the most pressing global challenges, with far-reaching environmental and societal impacts. To help address this crisis, Metal Organic Frameworks (MOFs) have emerged as promising materials for atmospheric water harvesting. Owing to their high surface area and exceptional ability to adsorb water, MOFs can significantly enhance water collection efficiency, even under low-humidity conditions. This study explores the synthesis and characterization of MIL-100(Fe) MOFs using two distinct approaches: a conventional solvothermal method and a greener synthesis conducted under milder conditions. It is noteworthy that the MOF obtained with the green synthesis (MMFe-G) exhibits a higher crystallinity and water adsorption capacity compared to its conventionally produced counterpart (MMFe), proving the potential advantages of greener synthesis strategies.

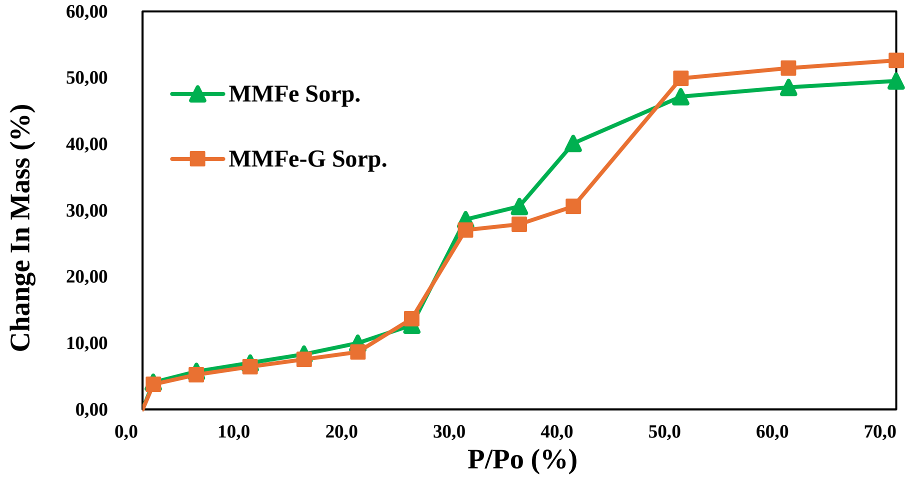

Figure 1. Water vapor adsorption isotherm (30 °C) for MMFe (□) and MMFe-G (**Δ**)

Characterization tests conducted on both materials indicate that the green approach can effectively reduce the environmental footprint of MOF production while maintaining, or even improving, water harvesting efficiency.

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FC3

Cellulose matrices amination towards the preparation of antimicrobial composites

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Cellulose is the most abundant natural material available on earth[1], non-toxic, biodegradable, biocompatible, and a renewable organic material, making it a good alternative to petroleum-based materials. The properties of cellulose make it interesting for the development of nanotechnology. For this very reason, it is often combined with metal nanoparticles for various biomedical applications, to research new antimicrobial agents, a global challenge due to microbial resistance to antibiotics (AMR). In particular, our studies concern the development of different cellulosic materials, such as cellulose paper or powder, functionalized with amino groups on the surface, with the aim to act as carriers for ZnO nanowires (ZnO-NWs), for the development of non-drug antimicrobial strategies. The introduction of amino pendants was associated with antibacterial properties, since cellulose does not have any antibacterial activity, which limited its application. Functionalization of cellulose via alkoxysilanes is one of the most efficient, environmentally friendly and safe ways to introduce a wide variety of functional groups[2]. The cellulose in the form of solid support or powder, such as cellulose paper or microcrystalline cellulose, were functionalized with various silane coupling agent including APTES (3-aminopropyltriethoxysilan) Different reaction conditions, and heating sources were tested obtaining a good grafting percentage. Moreover, different types of cellulosic material are under study, including cellulose derived from agri-food waste. The obtained materials were characterized by SEM-EDX, FTIR spectroscopy, X-ray diffraction analysis, and X-ray photoelectron spectroscopy. A direct disruptive mechanical interaction occurs with bacteria due to impaling with asymmetrical functionalized ZnO-NWs diffusing from the cellulose in presence of external stimuli (i.e. light)[3]. Finally, we will present preliminary results on the photocatalytic activity of the ZnO-NWs/amino-cellulose composites and their antimicrobial effects against both Gram-positive and Gram-negative bacteria strains.

Acknowledgements: The Italian Ministry of University and Research is acknowledged for funding through the PRIN 2022 project “Smart biopolymeric ZnO Nanowires composites for enhanced antibacterial activity (SOTERIA)” PNRR M4.C2.1.1. 2022WZK874 - CUP: H53D23004700006

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FC4

Polysaccharide-based film for a controlled release of indocyanine green for biomedical applications

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Biofilm formation on medical devices and infected wounds is one of the major causes of chronic infections in the healthcare sector[1]. Once biofilms form, they are often difficult to remove due to their high antibiotic resistance, endangering human life and health[2].

In the search for a suitable system to counteract this crucial issue, in the present study, we enriched a previously developed composite film based on chitosan (CS), sodium alginate (SA), and sodium carboxymethylcellulose (CMC)[3] with the phototherapeutic indocyanine green (ICG) dye to design a drug delivery system with antibiofilm features. Modulating the ICG concentration enabled obtaining different ICG aggregates through the porous structure of the polymer matrix, whose stability and release kinetics were evaluated in a medium that mimics physiological conditions. Infrared spectroscopy and X-ray diffractometry were used to obtain information regarding the interactions between the ICG dye and the polymer matrix, alongside its structural changes induced by different dye concentrations before and after dye release. We also investigated the macroscopic parameters of these films, such as swelling capacity, solubility, and the ability to absorb moisture, to explore their stability and integrity during application involving contact with an aqueous medium, packaging and storage. Lastly, the antibiofilm potential of the ICG-enriched films was assessed against *Staphylococcus aureus* ATCC 25923, displaying promising results for their future application.

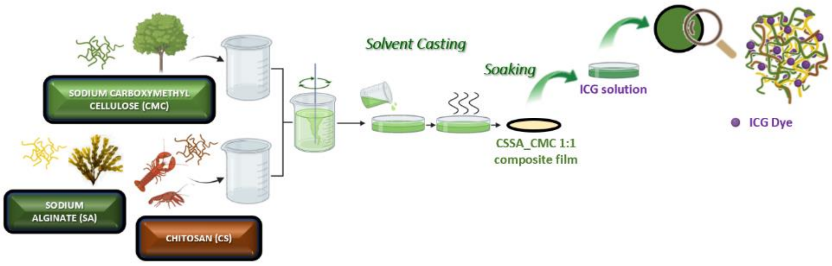

Figure 1. Preparation of polysaccharide-based composite film enriched with Indocyanine Green (ICG) dye.

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FC5

Ion exchange membranes for wastewater treatment

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Increased urbanization and industrialization have led to excessive consumption of natural resources followed by environmental pollution, including water pollution. Water is critical for the sustaining of the biotic components of ecosystems and living organisms, including humans. One of the objectives of the United Nations is to safeguard water resources in relation to sustainable development, and therefore guarantee the satisfaction of the needs of current generations without compromising the quality of life and the possibilities of future generations[1]. To deal with these problems, various technologies are used to purify water from contaminants. Chemical-physical decontamination methods such as chemical precipitation, coagulation, solvent extraction, ion exchange, adsorption with modified adsorbents and desalination techniques are encountered.

Among the methods mentioned, cation and anion exchange membranes play a key role in water treatment. They are distinguished by structure (homogeneous, semi-homogeneous and heterogeneous), material (organic and inorganic) and active group (cationic and anionic), therefore we can talk about selective ionic permeability. Properties, such as thermal stability, mechanical stability, and electrical conductivity, are defined by the material and functional groups. Recent progress concerns the synthesis of polymer-based membranes, generally composed of a single polymer chain and charged functional groups (positive or negative)[2].

The present work proposes two kinds of polymeric membranes for the removal of organic and inorganic species present in water: a sulfonated pentablock copolymer (s-PBC, commercially named Nexar™)[3] characterized by sulfonilic functional groups, and a new commercial polymer, named PTBr, containing quaternary ammonium groups. The physical and chemical properties of membranes were investigated by scanning electron microscopy (SEM), Fourier transform infrared (FT-IR) spectroscopy and X-ray photoelectron spectroscopy (XPS), while the removal efficiency, selectivity and kinetics towards different pollutants were evaluated by using the UV-VIS spectroscopic technique.

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FC6

Essential Oils in Sustainable Agriculture: Sol-Gel Microencapsulation for Prolonged Insecticidal Efficacy

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To become a truly sustainable alternative to synthetic pesticides, volatile and chemically unstable essential oils (EOs) such as those of *Citrus sinensis*, *Origanum vulgare*, and *Rosmarinus officinalis* showing strong *in vitro* insecticidal properties[1] need to be physically and chemically stabilized. Their application in open field indeed is limited by high volatility, chemical instability which require the use of high amounts of expensive essential oil with limited insecticidal efficacy. The sol-gel microencapsulation of EO within mesoporous, spherical silica microparticles ensures such physical and chemical stabilization, enabling the required prolonged release of the encapsulated actives.[2] Furthermore, contrary to hydrophobic molecules comprising most EOs, the hydrophilic SiO_2 microparticles functionalized with the EO can be formulated in water. In this presentation, we show how the sol-gel microencapsulation of *Citrus sinensis*, *Origanum vulgare* and *Rosmarinus officinalis* EOs can be readily achieved affords submicrometric, mesoporous spherical SiO_2 particles with a high loading capacity and high zeta-potential driving formation of stable dispersions in water. Controlled release experiments demonstrate the slow release of EOs over time, offering a promising alternative to conventional pesticides.[3,4] The sol-gel microencapsulation, furthermore, vastly enhances the biopesticide activity of the entrapped EO thanks to huge surface:volume ratio of the spherical, mesoporous SiO_2 microparticles. The excessive use of synthetic pesticides has become a major environmental and health problem, affecting ecosystems and human populations, with the spread of increased pest populations of more invasive species threatening global food security. The $45 billion synthetic pesticide industry manufactures over 3.5 million tonnes of synthetic pesticides used annually. These chemicals persist in soil and water, posing long-term health risks like neurodevelopmental disorders, cancer, asthma and many other ailments.[5] Additionally, synthetic pesticides contribute to environmental pollution, damaging wildlife and ecosystems. EOs are promising biopesticides whose practical application requires the aforementioned stabilization.

Acknowledgment

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FC7

Plastic pollution: Membrane Separation and Photocatalysis for the treatment of water effluents

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Plastic pollution is today a major environmental problem a global level. Of particular concern are micro- and nanoplastics due to their small size (diameter less than 5 mm for microplastics (MPs) and between 1 and 100 nm for nanoplastics (NPs). Recognized as "emerging" pollutants, MNPs have become a highly discussed topic in environmental research. With plastics now present almost everywhere, humans are exposed to a wide variety of micro and nanoplastics through inhalation, ingestion, and direct skin contact. Although the full effects of such exposure are not yet fully understood, potential risks include genetic modifications and alterations of the immune system. Aquatic environments are particularly vulnerable, as they act as key reservoirs where MNPs from various sources accumulate.[1]

In this study, an integrated and innovative technology[2] for the treatment of water contaminated by micro and nanoplastics was developed by combining membrane separation with a photocatalytic process. The membrane process allowed to concentrate the nanoplastics and microplastics contained in the treated aqueous streams, thus allowing to reduce the volume of wastewater to be subjected to the photocatalytic process. Key parameters such as permeate flux (J), fouling index (FI), cleaning efficiency (CE) and MNPs rejection were optimized in order to achieve high performance of the membrane process. Results showed that the membrane system achieved complete recovery of MNPs from real wastewater with complete restoration of the initial membrane performance, with a CE of 98% and a FI of 30%. The subsequently step of photocatalytic process using TiO_2 under UV light resulted in a degradation of MNPs as confirmed by total organic carbon and py-GC/MS analysis.

This approach highlights the potential of integrated systems as sustainable strategy to reduce the plastic pollution in aquatic environment and protect human health.

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FC8

Mechanistic Insights into the Reduction Process of Pt(IV) Complexes: From G-Quadruplex Binder Activation to Riboflavin-Mediated Photocatalysis

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Platinum(IV) complexes have garnered significant attention for their potential in anticancer therapy, representing a valid alternative to address the well-known disadvantages of traditional Pt(II) complexes. Pt(IV) prodrugs are more inert to ligand substitution than their Pt(II) counterparts and are less prone to deactivation before reaching tumor cells. Additionally, the axial ligands can be carefully selected to modulate both physical and chemical properties without altering the structure of the active pharmacophore. A critical step in the mechanism of action (MoA) of Pt(IV) complexes involves their reduction to Pt(II), which can occur either in the dark, through biological reducing agents such as ascorbate and cysteine, or be triggered by appropriate light irradiation.

In recent years, our group has extensively studied the mechanisms of action of Pt(IV) complexes using Density Functional Theory (DFT) calculations, enabling us to explore their reduction under both conditions.[1] Here, we present the results of two computational investigations. In the first, we focus on a Pt(IV)-salphen complex with chlorido ligands in axial positions, which, upon reduction by ascorbate or cysteine, releases the corresponding Pt(II) species capable of binding G-Quadruplex DNA.[2] G-Quadruplexes, non-canonical forms of DNA, have recently been identified as attractive targets in anticancer drug design. DFT calculations have been used to explore both inner- and outer-sphere reduction mechanisms involving classical reducing agents, while molecular dynamics simulations further reveal the key interactions responsible for G-quadruplex recognition.

In the second study, we investigate the photocatalytic activation of two Pt(IV) derivatives of cisplatin and carboplatin, both featuring carboxylate groups in axial positions, using riboflavin (Rf).[3] In recent years, Rf and its derivatives have been employed to activate Pt(IV) prodrugs through photo-reduction, leading to the release of clinically approved cisplatin and carboplatin. The mechanism of flavin-catalyzed reduction has been studied by means of DFT. First, we have examined the hydride-transfer mechanism between NADH and riboflavin under both dark and light conditions for the activation of riboflavin. Finally, we have explored the reduction of Pt(IV) by reduced riboflavin, comparing the results with those obtained using NADH and ascorbate to evaluate the conversion efficiency relative to commonly used bioreductants.

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FC9

Pathogen nucleic acid electrochemical detection for PCR-free sensing application

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Infectious diseases represent a crucial issue for worldwide public health, especially for those populations who live at low resource settings lacking of any appropriate lab and health assistance. In this scenario the PCR-free sensing is a very appealing and innovative approach providing the direct detection of the infectious pathogens without any complex molecular analysis due to the nucleic acid amplification or system architectures required by conventional PCR-based methods[1-3]. In this work we present a PCR-free sensing application of the protozoan Leishmania infantum, representative of pathogens affecting human health, based on the capacitive quantification of its pathogen nucleic acid kinetoplast (k)DNA through electrochemical impedance spectroscopy (EIS). Through its interaction with a self-assembled monolayer of oligonucleotide probes functionalized on top of a gold electrode surface, the kDNA target is directly detected and quantified without any amplification, thus, overcoming the time/cost-consuming procedures of conventional diagnostics.

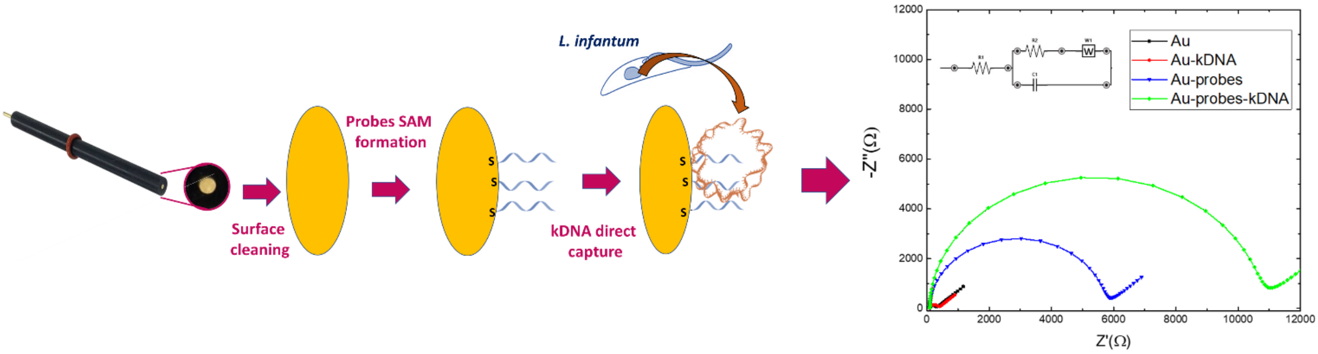

Figure 1. Gold sensing surface functionalization and EIS PCR-free detection of *L. infantum* kDNA.

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FC10

Electrochemical sensors for nitrate and ammonia ions detection in water

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Monitoring ammonium (NH_4^+) and nitrate (NO_3^-) levels in water is crucial due to their significant impact on environmental and human health. This work focuses on developing and characterizing sensitive, low-cost, and portable electrochemical sensors for real-time detection of these ions in water. Using screen-printing technology, electrodes with reproducible chemical performances can be developed. A screen-printed electrochemical cell is composed of three electrodes: working electrode (WE), reference electrode (RE), and counter electrode (CE). The inks used for printing determine the properties of the electrochemical cell, and the appropriate modification of the WE surface plays a key role in the development of sensitive and selective electrochemical sensors for molecules/target detection. Ammonium ions detection involved the use of conductive polymers and gold nanoparticles (Au NPs). The unique properties of polyaniline and gold nanoparticles enable efficient electrochemical signal transduction upon exposure to NH_4^+, leading to the accurate quantification of ammonium concentrations in water. Two strategies were employed using cyclic voltammetry (CV): electrodeposition of Au NPs on a commercial polyaniline/C electrode (Au/PANI/C) and CV-based electropolymerization of polyaniline on a commercial carbon electrode (Au/PANIep/C). The Au/PANI/C electrode exhibits excellent sensitivity at higher NH_4^+ concentrations (0.34 µM limit of detection, LoD) but decreases sensitivity at lower concentrations (0.01 µM LoD). Conversely, the Au/PANIep/C electrode shows better performance for low NH_4^+ concentrations (0.03 µM LoD) and lower sensitivity for higher concentrations (0.07 µM LoD). Both electrodes shows good reproducibility, with a maximum relative standard deviation (RSD) of 3.68% for Au/PANI/C and 5.94% for Au/PANIep/C [1].

Nitrate ions detection involved the use of copper (Cu) due to the high conductivity (5.8×10^7 S/m), which improves charge transfer. Cu micro-flowers were electrodeposited on a carbon WE using CV. This sensor exhibits a sensitivity of 44.71 µA/mM, a low detection limit of 0.87 µM, and a dynamic linear range from 0.05 to 3 mM. Additionally, the NO_3^- sensor shows good stability (maximum RSD of 5% after ten measurements), reproducibility (maximum RSD of 4%), and repeatability (RSD of 5.5% after ten measurements) [2]. These results highlight the potential of the developed sensors for effective monitoring of NH_4^+ and NO_3^- in water, contributing to enhanced water quality management and environmental protection.

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FC11

Enhancing the photoluminescence of citrus-derived Carbon Quantum Dots through Experimental Design

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Carbon Quantum Dots (CQDs) are photoluminescent carbonaceous nanomaterials characterized by a particle size smaller than 10 nm and the presence of hybridized sp^2 carbon and oxygen-containing groups on their surface.[1] The synthesis of CQDs from green sources, such as biomasses, offers a promising alternative for waste management, enabling the reuse of agricultural and food industry wastes. This approach has gained significant attention due to the biocompatibility, sustainability and cost-effectiveness of the starting materials.[2] Among various preparation strategies, the most common is the green hydrothermal method. However, there is considerable variation in the literature regarding the optimal synthesis conditions. For hydrothermal treatment using water as solvent, temperature, time, and initial concentration of precursors influence the particle size, surface functionalization and, consequently, the photoluminescence properties and stability of the CQDs.[3]

This work exploits the chemometric tool of experimental design[4] to optimize the synthesis of biomass-based CQDs. Citrus waste bergamot pomace was used as a precursor. An initial hydrothermal synthesis was carried out using 250 mg of pomace in 25 mL of water, heated in an autoclave at 180 °C for 6 hours.[5] The experimental design was then conducted according to a 2^k full factorial design while varying the initial amount of precursor, the temperature, and the reaction time. After purification, the quantum yield was measured using quinine sulfate as a reference. The results were used to construct the experimental surface, allowing to determine the optimal conditions for the synthesis of CQDs.

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FC12

Metal release from perovskite solar cells: environmental risk assessment by voltammetric analysis

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Perovskite solar cells (PSCs) are a promising alternative for photovoltaic power generation, but the toxic materials used in their synthesis can pose environmental and health risks. While encapsulation helps prevent the release of hazardous substances, extreme weather events (hail, snow, fires) or improper waste disposal can damage the cells, leading to potential exposure[1]. The degradation of perovskites represents a significant challenge for their stability. Several studies suggest that the degradation process may start with the formation of hydrated compounds on the surface of the material, which then propagate into the film. Some suggest that degradation occurs in two distinct phases and is strictly dependent on the presence of water[2]. To overcome these problems, various solutions have been proposed. The use of bromides has been suggested to strengthen the hydrogen bonds in the film between $CH_3NH_3^+$ and $[PbI_6]^{4-}$, thus avoiding the formation of hydrated compounds. O_2 can influence degradation by oxidizing organic material, especially in the presence of light. Perovskite degradation results in the formation of starting materials, such as PbI_2, small amounts of metallic lead and carbonate compounds. Hydroiodic acid and methylamine can be formed by reacting with carbonic acid. Lead tends to strongly adsorb onto soil particles. HI can acidify soils, promoting the dissolution and migration of metal ions and halides, increasing the risk of contamination. Voltammetric techniques[3] have proven useful for quantifying several analytes due to their intrinsic sensitivity in distinguishing between different redox species and labile metal complexes. These techniques have been used to evaluate lead release from PSCs, also due to the rapidity of the method. The stability of the perovskite cells and the risks of lead release were assessed by leaching experiments in distilled water.[4] The concentration of Pb in the leachate was measured by anodic stripping voltammetry, using a polarograph with a mercury drop electrode, a reference electrode with Ag/AgCl and a platinum counter electrode. The analyses compared devices with and without surface electrodes. The electrodeless perovskite released higher amounts of Pb^{2+}, while the presence of an evaporated electrode reduced the release, thanks to the greater stability provided by the oxides and metal layers acting as a barrier against degradation in the aqueous phase.

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FC13

An eco-friendly analytical approach for lithium battery recycling

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In recent decades, the demand for lithium-ion batteries (LIBs) has grown significantly due to the increase in global energy consumption. The increase of batteries market corresponds to an intensification in their production and consequently more spent batteries to be disposed of.[1] Landfill disposal releases harmful substances into soil and groundwater, contributing to environmental pollution. These reasons, combined with difficulties in supply of raw materials for LIBs production, lead to the need to recycle batteries at their end of life.[2] The most common recycling techniques include pyrometallurgical and hydrometallurgical processes, which have important limitations related to hazardous gases emission, high energy consumption, and unsafe adopted solvents.[3]

The analytical approach proposed in this research project is aimed at recovering valuable metals from spent batteries through a sustainable method. The developed procedure consists in the extraction of metals from the black mass (BM), a black powder obtained by grinding whole batteries, at their end of life, and containing all their components: metals, graphite and organic polymers. Leaching was performed using eco-friendly solvents at room temperature and pressure, under controlled time conditions, and evaluating the extraction efficiencies of three different mixtures. Metal leaching is performed under different conditions: strong, mild, and mild/mixed. The adopted experimental protocols were combined with instrumental analysis, such as LDI-MS, to establish the presence of PVDF polymer, and ICP-MS, to assay metal cations in BM residue and in cation-enriched solution.

The results obtained showed that the adopted methods allow the recovery of the metal cations Ni, Co, Li, Mn, Cu, Al, Fe, Zn and Mg. Leaching with the extraction mixture under strong conditions resulted in extraction efficiencies above 90% for all metals after 168 hours, except Mg. The mild system yielded extraction efficiency over 80% only for copper and iron. Extraction with the mild/mixed solvent system led to metal concentrations in solution ten times higher than under mild conditions, giving promising results. Results, comparable to those under strong conditions, could be achieved with less impact on the environment by optimizing leaching time and solvent ratios in mild/mixed system.

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FC14

Sulfur-Functionalized Single-Walled Carbon Nanotube Buckypaper/MTV-BioMetal−Organic Framework Nanocomposites for Gold Recovery

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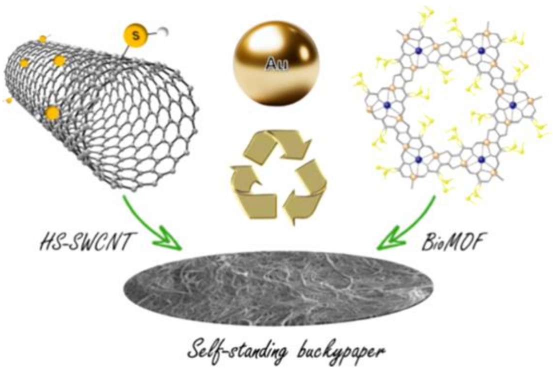
Developing sustainable, efficient, and selective gold recovery technology is essential to implement the valorization of complementary alternative sources for this precious metal, such as spent e-waste, and to preserve the environment. The main challenge in recovering gold from liquors obtained from leached waste electronics is the low concentration of Au compared to impurities. Here, we report the preparation of a novel multivariate biological metal−organic framework (MTVBioMOF) incorporated within single-walled carbon nanotube buckypapers (SWCNT-BP) to yield an MTV-BioMOF@HS-SWCNT-BP composite, as a potential material for the selective recovery of gold metal ions from water[1]. The thiol-functionalized SWCNT-BP surface and the presence of thioether groups evenly decorating the MTV-BioMOF channels shape a task-specific functional environment that boosts the interactions with gold metal ions, reaching efficiency values of gold recovery up to 99.5%. This high recovery efficiency, with values as high as 98.0%, is maintained even in the presence of competing metal cations, also demonstrating a noticeable selectivity. This composite material represents a promising paradigm for the selective extraction, enrichment, and purification of gold.



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FC15

Nutritional profile and antioxidant capacity of plant-based kefir milks

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The growing interest in fermented dairy products is due to their health-promoting properties. The use of milk kefir grains as a starter culture has led to products with different nutritional and biological profiles depending on the type of milk[1]. Most research on kefir has focused on milk substrates of animal origin, especially cow milk [2]. An alternative way to intake beneficial health effects from kefir is through of its adaptation to non-dairy substrates for the production of new probiotic products to provide vegan, lactose intolerant, and dairy-product allergic consumers[3]. Thus, plant-based milks were used as medium of kefir fermentation. Almond, coconut, hazelnut, oat, rice, soy, walnut milks were inoculated with 10% (*w/v*) milk kefir grains for 24 h at room temperature.
The fermentation led to an increase of protein content in all samples, except soy one where it was reduced and walnut sample for which it remained unchanged. Beneficial fatty acids such as oleic and linoleic acid rose in all samples. Total phenolic content (TPC), determined by the Folin-Ciocâlteu method, increased during fermentation in all samples: kefir from walnut milk showed the highest TPC (350.9 ± 3.0 µg GAE/mL) followed by soy sample (337.2 ± 8.4 µg GAE/mL).
Fermented beverages highlighted a better antioxidant profile compared to the corresponding unfermented samples at the highest concentration. The antioxidant activity was evaluated by ferric reducing antioxidant power (FRAP) and ABTS assays.
The results showed improved activity in all fermented milks being highest in almond sample, both against ABTS (44.9 ± 1.5 $\%I_{ABTS}$) and FRAP test (536.0 ± 1.0 µM $FeSO_4$/mL). The adaptation of milk kefir grains into different substrates, such as plant-based milks, represents a promising avenue for the production of innovative beverages to be potentially consumed as a promising probiotic alternative.

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FC16

Recovery of spent lithium ion batteries for catalytic biomass upgrading

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The generation of spent lithium-ion batteries (s-LIBs) worldwide amounts to millions of tons annually. While current recycling methods focus on extracting valuable metals like Ni, Co, and Li, they suffer from poor selectivity, high energy requirements, and expensive by-product management. Consequently, there's growing interest in exploring alternative methods for the direct reuse of s-LIBs [1]. At the same time, lignocellulosic and agro-industrial waste and residues represent a central feedstock for modern biorefineries aimed to the sustainable production of renewable energy and biobased materials and chemicals [2]. Technologies such as hydrothermal carbonization (HTC) have been proposed to upgrade orange peel waste (OPW), yielding hydrochar (OPW-HC) and liquid bio-oil (OPW-OIL), rich in furans derivatives like furfural and 5-HMF, pivotal in modern biorefineries [3]. OPW-OIL can be very rich in furans derivatives (furfural and 5-HMF) that represent one of the most important classes of intermediates in modern biorefineries.

Starting from these two abundant wastes, we propose a simple direct approach to transform the s-LIBs into an efficient cobalt-based heterogenous catalyst. This catalyst has demonstrated excellent efficiency in the upgrading reactions of biomass derivatives

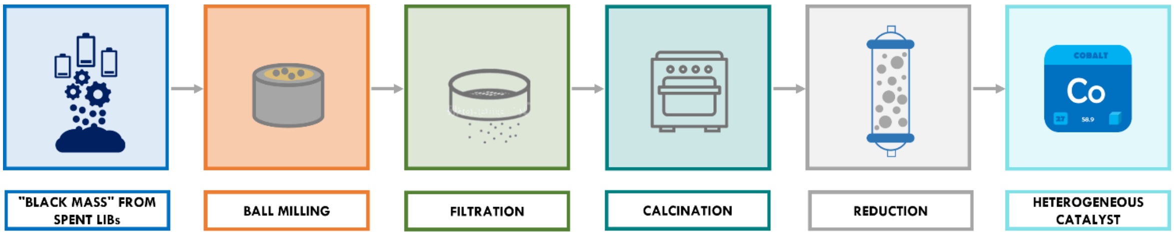

Figure 1. Schematic representation of the mechano-thermal treatment of spent LIBs "black mass" for the preparation of Co-based heterogenous catalysts

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FC17

Harnessing Nanotechnology: Boosting Solar Cell Performance with Quantum Dots and Gold Nanoparticles

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It has engineered quantum solar cells (i.e., with traditional quantum dots, QDs, and carbon quantum dots, CQDs) with a focus on the refinement of light absorption and charge carrier separation and probing innovative concepts such as multiple exciton generation to boost overall device efficiency.
An optimization study on dye-sensitized solar cells (DSSCs) utilizing both synthetic and natural dyes was conducted through a meticulous synthesis process that involved incorporating gold nanoparticles into a TiO_2 semiconductor and refining the particle sizes of the TiO_2 in the scattering layer (Fig. 1). Noble metal nanostructures are recognized for their unique properties derived from surface plasmon resonance[1], which has been applied across various fields such as sensing, photocatalysis, optical antennas, and photovoltaic devices. By integrating gold nanoparticles into the mesoporous TiO_2 layer and introducing a scattering layer, we enhanced the power conversion efficiency (PCE).
During these experiments, we observed promising results in terms of light absorption and charge transfer efficiency, which are crucial parameters for the improved performance of solar cells. This will lead to a significant advancement in photovoltaic technologies and promote the scalable use of QDs in energy harvesting applications.

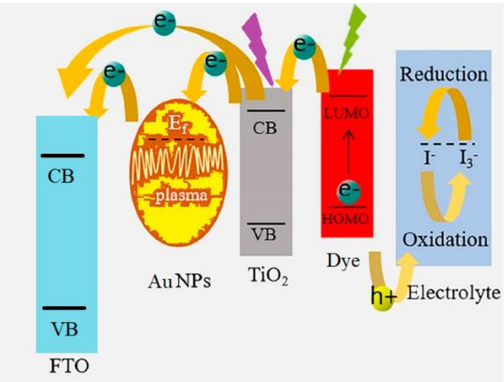

***Figure 1**. Cross-section view of plasmonic-based dye-sensitized solar cell[1]*

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FC18

Evaluation of tetrahydropyrrolo[3,4-*c*]pyrazole derivatives as sigma-1 receptor ligands

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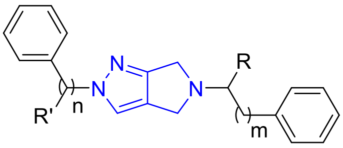
Sigma receptors (SRs) composed of two subtypes − sigma-1 (S1R) and sigma-2 (S2R) − are chaperone transmembrane proteins classified as non-G protein-coupled receptors. They are primarily located in the endoplasmic reticulum membrane, forming physical associations with the mitochondria.[1] SRs have attracted increasing interest for their emerging roles in neurodegenerative diseases and their potential in modulating neuropathic pain (NP).[2,3] In this study, we designed and synthesized novel S1R ligands based on the tetrahydropyrrolo[3,4-*c*]pyrazole scaffold (Figure 1). This rigid and versatile heterocycle enhances key properties of the ligands, particularly their potential interaction with S1R, by improving the molecular shape and electronic distribution. Structure-activity relationship (SAR) studies revealed that substitutions on the nitrogen atoms are crucial in modulating S1R binding affinity. Among the synthesized compounds, AD417 exhibited a nanomolar affinity for S1R (K_i = 75 nM) and a marked selectively over S2R (K_i = 431 nM). Moreover, AD417 demonstrated minimal inhibition of the hERG channel (IC_{50} = 5.8 μM), indicating a favorable safety profile. Molecular modeling studies provided insights into the observed SAR, elucidating the key interactions responsible for ligand affinity and selectivity. These findings highlight the potential of tetrahydropyrrolo[3,4-*c*]pyrazole derivatives as selective SR modulators, offering promising avenues for developing more effective and safer therapies targeting S1R, particularly in NP treatment.

AC28, n = 2, m = 0, R = CO_2Et, R' = H
AC31, n = 3, m = 0, R = CO_2Et, R' = H
AC35, n = 1, m = 0, R = CO_2Et, R' = H
AC46, n = 4, m = 0, R = CO_2Et, R' = H
AC49, n = 3, m = 1, R = CO_2Et, R' = H
AC54, n = 0, m = 1, R = CO_2Et, R' = H

K_i S1R 🔴
K_i S2R 🔴

AC38, n = 3, m = 0, R = $CONEt_2$, R' = H

K_i S1R 🟠
K_i S2R 🔴



affinity scale 🔴 < 🟠 < 🟡 < 🟢 < 🟢

AD417, n = 1, m = 1, R = H, R' = $CONEt_2$

K_i S1R 🟢
K_i S2R 🟡
IC_{50} hERG = 5.8 μM

AD457, n = 1, m = 2, R = H, R' = $CONEt_2$

K_i S1R 🟠
K_i S2R 🔴

Figure 1. Structures and biological data of tetrahydropyrrolo[3,4-*c*]pyrazole-based derivatives.

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FC19

RESCUING P53 BY NEW TRANSLATIONAL READTHROUGH INDUCING DRUGS

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Nonsense mutations represent a distinct category of mutations, characterized by converting an amino acid coding triplet into a premature termination codon (PTC). This results in a notable reduction in cytosolic mRNA levels, ultimately leading to the premature halting of translation and the production of truncated and non-functional proteins. A substantial number of genetic disease (11%) and hereditary tumor (12%) is attributable to nonsense mutations. In this respect, TP53 represents one of the most frequently mutated genes[1]. The protein encoded by TP53 is p53, a transcription factor designated as "the guardian of the genome" due to its role in maintaining the integrity of the cell genome. p53 performs many functions within the cell, including regulating cell cycle progression, DNA repair, apoptosis, and senescence. It is estimated that over half of all human cancers exhibit mutations in TP53, with 10% of cases resulting from nonsense mutations. This highlights the urgent need to develop innovative therapeutic strategies[2]. One strategy in nonsense mutation treatment is based on the pharmacological induction of translational readthrough (RT). This process involves suppressing a stop codon using translational readthrough-inducing drugs (TRIDs)[3]. In the present work, we developed a novel pharmacophore model using a ligand-based approach to identify potential TRIDs capable of restoring the expression of a complete p53 protein. Following the synthesis of these new compounds, their capacity to induce translational readthrough was evaluated using a Firefly luciferase (FLuc) assay in HeLa cells with a nonsense mutation. The best-performing molecules were evaluated for their effectiveness in producing full-length p53 protein.

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FC20

Preliminary Results about the Structural Characterization of Chickpea β-chain Legumins: An integrated Bottom-up and Top-down proteomic approach

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Chickpea is an important food legume crop with high protein levels and a lot of functional properties and health benefits, which includes reducing cardiovascular, diabetic, and cancer risks.[1] These properties lead this legume an interesting component for the development of protein-enriched foods.[2] On the other hand, a number of people are allergic to chickpea and its possible association with IgE-mediated hypersensitivity reactions, especially among children, merits serious attention. Particularly, the most abundant proteins of chickpea seeds are legumins and vicilins, a group of storage proteins that accumulate to high levels in seeds during the late stages of seed development, and are degraded during seed germination. The resulting amino acids are utilized by the developing seedlings as a nutritional source. Legumins and vicilins, belonging to the cupin superfamily, have been already shown to resist both in vivo and in vitro digestion, and are described as having allergenic properties.[3,4] Particularly, one of the major chickpea allergens was identified as the basic subunit (β-chain) of legumins.[5] Taking into account that these proteins represent the major components in grains and, of the plant proteins, represent those that are the most abundantly consumed by humans, a detailed structural characterization of their sequence is needed. Here it is reported an integrated bottom-up and top-down approach aimed to the structural characterization of chickpea β-chain legumins. The preliminary results allowed the detection and characterization of different proteoforms of chickpea β-chain legumins.

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FC21

Bolaamphiphiles *via* sulfenic acid

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Bolaamphiphiles or two-headed amphiphiles are molecules characterized by a hydrophobic skeleton joined to two hydrophilic heads.[1] They are interesting systems for the unique property of self-assembling both at interfaces (*e.g.* air/water or liquid/solid) and in solution, forming a wide variety of well-defined structures (micelles, lamellae vesicles, nanotubes, nanorods, and nanosheets). In this communication the synthesis of some sugar-decorated bolaamphiphilic molecules (Figure 1), performed following an original pathway, is described.[2] The central aromatic platform was obtained from the reaction of a suitably substituted bis-sulfoxide with diethynyl benzene. In particular, the intermediates of such reactions are sulfenyl derivatives that easily react with a triple bond to give vinyl sulfonyl moieties.[3,4] The functionalization at the terminal triple-bonds of the central core, performed by a copper-free Sonogashira cross-coupling, allows the introduction of different carbohydrates units. Finally, the vinyl-sulfonyl functions in the aromatic platform, representing two efficient Michael acceptors, favor further modification of these structures, opening the route to original molecules with different physical properties and self-assembly characteristics.

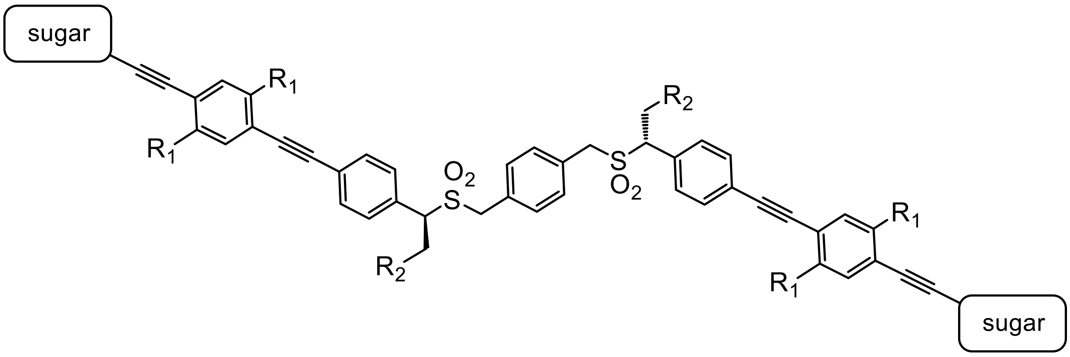

Figure 1. The skeleton of synthesized sugar-functionalized bolaamphiphilic molecules.

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FC22

Chirality influences the biological properties of novel NHC-gold and -silver complexes.

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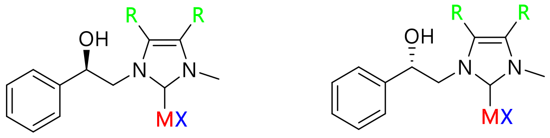
NHC-gold and -silver complexes have drawn the interest of several researchers because their chemical versatility and multiple biological properties[1]. However, most of these complexes contain one or more chiral centres and the studies have usually been carried out on the racemic mixture. Thus, many questions about how the chirality may influence the biological and medicinal properties remain still unanswered[2]. Aiming at a better understanding, herein a series of enantiopure NHC-gold and silver complexes was synthesized, characterized and biologically evaluated through different *in vitro* systems. The leads exerted different properties depending on the complexed metal and the configuration of the stereocenter, being the (*R*)-gold NHC complexes the most active, particularly as anti-inflammatory molecules. Docking simulations supported the *in vitro* results, indicating a different binding mode to the individuated target for the considered enantiomer. Moreover, the anticancer and antibacterial activities were also studied for each enantiomer. Overall, the reported data contribute to a better understanding of the different biological properties exerted by the enantiopure complexes.



(S)-AgL1 R=H; M=Ag; X=I	(R)-AgL1 R=H; M=Ag; X=I
(S)-AgL2 R=Cl; M=Ag; X=I	(R)-AgL2 R=Cl; M=Ag; X=I
(S)-AuL1 R=H; M=Au; X=Cl	(R)-AuL1 R=H; M=Au; X=Cl
(S)-AuL2 R=Cl; M=Au; X=Cl	(R)-AuL2 R=Cl; M=Au; X=Cl

Figure 1. Structures of the studied enantiomerically pure NHC-gold and -silver complexes.

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FC23

Oxidative carbonylation of β-amino alcohols catalyzed by Pd supported on silica-POSS-Imi

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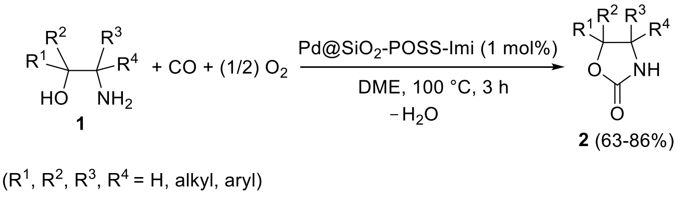
The direct synthesis of 2-oxazolidinones by the oxidative carbonylation of *β*-amino alcohols[1] allows obtaining high value added molecules with several biological applications. 2-Oxazolidinones are known, in particular, to possess significant antibacterial[2] and antitumor activities.[3]

We have now found that it is possible to perform this kind of transformation by supporting our PdI_4^{2-} catalyst (already widely applied in the development of oxidative carbonylation processes under homogeneous catalysis conditions)[4] on a hybrid material based on imidazolium modified polyhedral oligomeric silsesquioxanes (POSS-Imi) grafted on amorphous silica (SiO_2).

The newly developed heterogeneous catalyst was proved effective with a wide range of *β*-amino alcohols **1** to give the 2-oxazolidinone derivatives **2** in fair to high isolated yields (63-86%) as shown in **Scheme 1**.

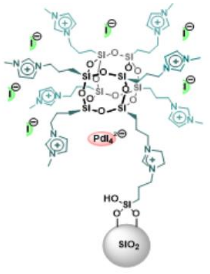


1

2 (63-86%)

(R^1, R^2, R^3, R^4 = H, alkyl, aryl)

Scheme 1



Pd@SiO$_2$-POSS-Imi

The recyclability of the catalysts has been successfully verified for three consecutive runs.

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FC24

Structural characterization of the protein fraction extracted from extracellular vesicles secretes by astrocytes using high-resolution mass spectrometry

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Parkinson's disease (PD) is a neurodegenerative disease caused by the progressive loss of dopaminergic (DAergic) neuronal cell bodies in the ventral midbrain (VMB) and their terminals in the striatum (STR). Astrocytes (AS) play a crucial role in maintaining the homeostasis of DAergic neurons, and extracellular vesicles (EVs) secreted by astrocytes (AS-EVs) can have either destructive or beneficial effects[1]. To identify the mechanisms involved in the neuroprotective effects of AS-EVs, we have characterized their protein fraction and specific post-translational modifications (PTMs), comparing vesicles secreted by AS from the VMB vs. the STR, both in basal conditions (AS-EVs CTRL) and activated by the pre-treatment with the neuroprotective chemokine CCL3 (AS-EVs CCL3)[2].

Intact EVs were purified from primary cultures of postnatal VMB and STR astrocytes. EVs were lysed using 0.1% RapiGest SF and proteins were reduced with DTT, alkylated with iodoacetamide and digested using trypsin. Analysis was conducted in triplicate by a shotgun approach and nanoUHPLC/High-Resolution nanoESI-MS/MS[3].

MS analysis revealed a different protein profile and a different pattern of PTMs in AS-EVs CTRL and AS-EVs CCL3 extracted from VMB and STR. In particular, we focused the attention on PTMs related to protection and degradation pathways of proteins as ubiquitination, oxidation, succination, phosphorylation and deamidation. The assignment of functional roles to these PTMs will be a further step towards the full understanding of the impact of EVs on neurodegeneration.

Overall, our study suggests the existence of a molecular machinery capable of organizing the sorting of specific proteins towards EVs in nigrostriatal astrocytes. Furthermore, it implies the possibility that secreted proteins with specific PTMs may have specific functions when transferred to target cells and thus the reprogramming of AS-EVs as a novel strategy for brain repair. Finally, the knowledge generated within this study may pave the way for the development of innovative therapeutic approaches to tackle PD.

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Poster

PO1

Screen-Printed Carbon Electrode (SPCE) modified with supramolecular assembly of graphene cyclodextrin and ferrocenyl-carnosine for Mn(II) electrochemical sensing

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Manganese is an essential nutrient for the human body, but it can exhibit symptoms of neurotoxicity at high levels. The Environmental Protection Agency (EPA) has set a maximum allowable level of 0.05 µg/mL in drinking/domestic water. Considering the importance of the strict monitoring of manganese at low concentrations in water samples, we have exploited the combination of the electrical properties of a graphene nanoplatform derivatized with mono-6-deoxy-6-azido-β-cyclodextrin as well as the complexing abilities and electroanalytical properties of ferrocenyl-carnosine (FcCAR)[1] for the electrochemical detection of Mn(II). The voltammetric response of the graphene nanoplatform derivatized with mono-6-deoxy-6-azido-β-cyclodextrin film-modified Screen-Printed Carbon Electrode (SPCE) was first investigated by Cyclic Voltammetry (CV) using $K_3Fe(CN)_6$ as a redox probe. Then, the electrochemical behaviour of FcCAR on the modified SPCE was studied in the absence and presence of the metal by CV and Differential Pulse Voltammetry (DPV). This system showed a 2.4-fold higher signal than that of the bare SPCE and high performance in the presence of Mn(II) with a sensitivity of 0.016 µA/nM, while the Limit of Detection (LOD) and Limit of Quantification (LOQ) were 0.48 nM and 1.59 nM, respectively. These results are certainly encouraging compared with those reported in the literature[2,3].

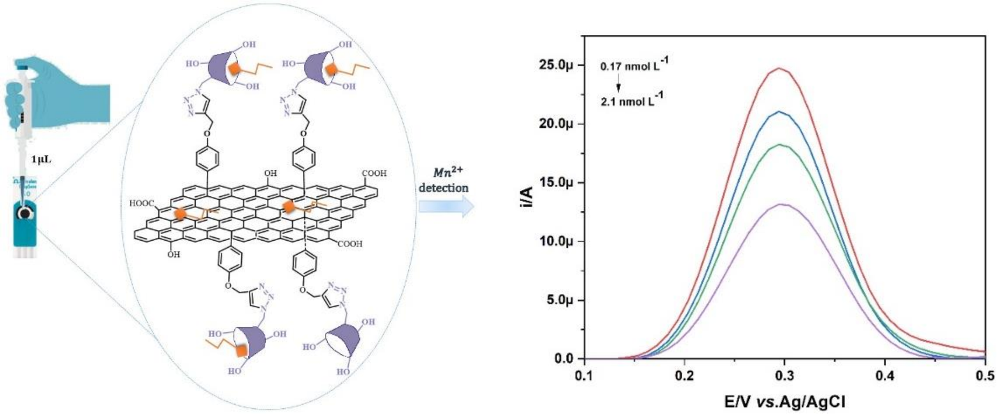

Figure 1. Representative scheme of the experimental procedure.

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PO2

Non-Enzymatic Electrochemical Sensors for Glucose Detection Based on Metal Oxides

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Glucose sensors play an important role in managing blood glucose levels of diabetic patients [1]. Furthermore, as a component of more complex structures such as polysaccharides and glucosides, glucose plays an important role in energy storage and as components of plant cell walls.[2] Among several techniques, electrochemical detection has been broadly applied due to its high selectivity, sensitivity, simplicity and low cost.[3] Although enzyme-based glucose test strips dominate the glucose detection market, the intrinsic chemical and thermal sensitivity of enzymes stimulates researchers to explore chemically and thermally stable metal oxides as alternative sensing materials for non-enzymatic glucose detection. The electrochemical signals encompass electron transfer in the electrode, induced by reactions occurring at the electrode-electrolyte interface. This work begins with sensing mechanisms and working principles of metal oxides-based glucose sensors, followed by the discussion of metal oxides based non-enzymatic glucose detection. Metal oxides were synthesized by the hydrothermal method, to obtain electrode materials exhibiting enhanced and optimized electrochemical performance towards detections of glucose. The structure and morphology were characterized by Scanning Electron Microscopy (SEM) and X-ray diffraction (XRD) analyses. Electrochemical tests for glucose sensing were performed in alkaline environments using Cyclic Voltammetry (CV), Differential Pulsed Voltammetry (DPV) and Amperometry.

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PO3

Polymer-lignin hybrid films for Methylene Blue degradation in aqueous solutions

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There is a growing need for new efficient water and soil adsorbents based on biopolymers. Since lignin is rich in functionalities,i.e. hydroxyl, methoxyl and carboxyl functional groups, it can be used as an adsorbent for the removal of various pollutants[1]. However, due to its heterogeneity, recalcitrance and the lack of a solvent system for lignin, it is difficult to use it as a polymeric material. To this end, lignin (L) dissolved in polyethylene (glycol) (PEG) was chemically cross-linked with poly(vinyl alcohol) (PVA) and polyvinyl pyrrolidone (PVP), which are biodegradable synthetic polymers. The effect of the lignin and sodium oleate (SO) content in polymer matrix and the physicochemical properties of the PVA-PVP-L films were evaluated. Studied films have exhibited 50 to 87% methylene blue (MB) degradation within 2 h. The results of the FTIR spectra analysis of the pristine films and after dye adsorption show changes due to the attachment of MB, revealing characteristic IR adsorption bands of MB at 1390 and 1330 cm^{-1}, corresponding to $-CH_3$ symmetric deformation and C=N bond, respectively. Furthermore, upon interaction with MB, the peak at 3500-3100 cm^{-1} was shifted to a lower wavelength, indicating that the phenolic hydroxyl group is the main reaction site for MB adsorption[2]. These phenolic hydroxyl groups can form active hydrogen bonds with MB molecules. These observations suggest that the methylene blue molecules were preferentially adsorbed on the surface of the PVA-PVP-L films by electrostatic interaction, but additional hydrogen bonding also took place.

Acknowledgments

Thanks are due to the Circular and Sustainable Made in Italy Extended Partnership (MICS) funded by the European Union Next-Generation EU (Piano Nazionale di Ripresa e Resilienza (PNRR) - Missione 4, Componente 2, Investimento 1.3 - D.D. 1551.11-10-2022, PE00000004) for financial support".

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PO4

In silico-guided discovery of novel Sortase A Inhibitors

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Sortase A (SrtA) is a bacterial cell membrane enzyme responsible for anchoring key virulence factors to the cell wall surface of Gram-positive bacteria, acting as a critical driver of their pathogenicity. Its membrane localization makes it an accessible and appealing target for the development of novel antivirulence drugs, which could be useful in combating the rise of bacterial drug resistance.[1]

In this work, virtual screening studies were conducted to identify novel SrtA inhibitors. Starting from the PDB structure of SrtA (PDB code: 2KID),[2] molecular modeling analysis guided the identification of new potential SrtA inhibitors. The receptor structure and the ZINC20 database[3] were prepared using the Protein Preparation Wizard and LigPrep tools,[4] respectively. The docking studies were performed by means of Glide v.8.9 SP algorithm.[4] Finally, 7 compounds were selected and purchased. Biological assays confirmed the ability of two compounds to effectively inhibit SrtA activity. Extensive experimental tests are currently underway.

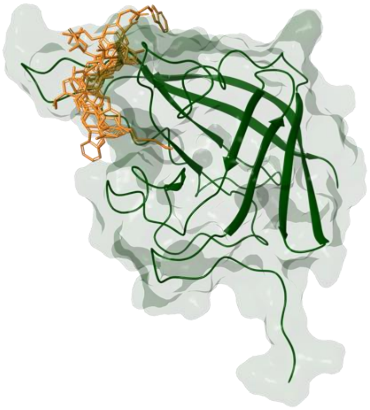

Figure 1. 3D representation of SrtA and the best selected compounds. The enzyme and the ligands are showed as forest cartoon and orange sticks, respectively.

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PO5

Molecular Dynamics simulations of the permeation of statins across lipid membranes

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Among the multiple anticancer therapies that can be applied, chemotherapy is the most adopted and, sometimes, the only one appliable, as in the case of cancer in advanced stages. However, one of the most relevant drawbacks that affect actually applied anticancer drugs is their inability to discern between cancerous and health cells, determining various side effects. In this computational work the interaction between two lipophilic statins, Simvastatin and Fluvastatin (Figure1), and plasmatic membrane models of normal and cancer cells was examined aiming at evaluating their impact and differential behavior. Statins, consolidated to treat hypercholesterolemia and cardiovascular disease, were chosen because in the last years they are in repositioning phase as possible adjuvants of different anticancer drugs. [1-3] In addition, statins can modify structural properties of cell membranes with an impact on their functioning. Despite this knowledge, due to the complexity of the systems, the precise mechanism by which statins induce apoptosis in tumor cells has not yet been fully understood and needs other clarifications. For this reason, the investigation of the crossing by passive diffusion of different membrane typologies, obtained by applying molecular dynamic (MD), could provide useful information about the real-life behavior of drug-membrane systems that cannot be obtained experimentally, or that is too expensive to obtain in terms of time and resources. Here the outcomes of a MD exploration of statin-membrane interactions and of the effects statins can have on various structural and chemical-physical parameters are illustrated.

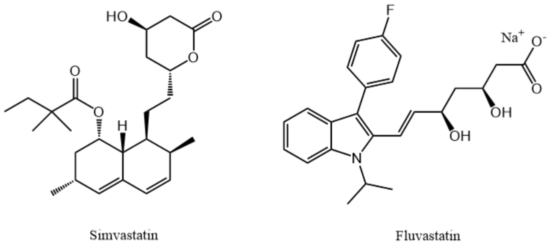

Figure 1. Chemical structures of the two statins considered in this study.

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PO6

Novel Approach for Detecting Hemoglobin Imbalance in Human Plasma Using a Fluorescent Schiff Base-Modified Nanocellulose Chemosensor.

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Recently, the challenge of developing of new fluorescent turn on/off chemosensors has attracted significant interest due to the sensitive and selective detection of biologically important metal ions.[1] This work has developed a new, rapid, highly sensitive, and precise approach to identify the imbalance level of hemoglobin through fluorescence emission spectroscopy. Among all the identified fluorescent materials, Schiff base ligands have been extensively studied for sensing cations and anions due to their potential to form stable complexes and their easy one-step synthesis.[2] A study on a new Schiff base modified nanocellulose (PY-PDA-DANC) applied as a fluorescent chemosensor is reported. To prepare the chemosensor, nanocellulose (NC) was first converted into 2,3-dialdehyde nanocellulose (DANC), and then modified by grafting o-phenylenediamine (PDA), followed by 1-pyrenecarboxaldehyde giving rise to the new blue fluorescent complex PY-PDA-DANC. All the synthesized products were characterized using FTIR, ^{1}H NMR, XRD, EDX and UV–vis spectroscopy. The fluorescence response of PY-PDA-DANC against various metal ions (Co^{2+}, Cr^{3+}, Cu^{2+}, Fe^{2+}, Fe^{3+}, Hg^{2+}, K^+, Mg^{2+}, Mn^{2+}, Na^+, Ni^{2+}, Pb^{2+} and Zn^{2+}) in DMSO/H_2O media was evaluated using PL spectroscopy. The fluorescent sensor showed high and selective quenching response to Fe^{2+} ions with low limit of detection (LOD). PY-PDA-DANC was also successfully applied for sensing of heme–iron coordinated to hemoglobin (HB), displaying a LOD of 28.45 nM. Subsequently, it was applied for the analysis of [Fe^{2+}@HB] in human plasma sample with good recoveries.

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PO7

Innovative *In Silico* Method for Discovering Multi-Target JAK/STAT Inhibitors as Potential Anticancer Therapies

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The JAK/STAT signaling pathway regulates key cellular processes such as immune modulation, cellular proliferation, and apoptosis. Its dysregulation is implicated in various cancers, making it an attractive target for anticancer therapies[1]. In this study, we present an innovative *in silico* strategy to identify multi-target inhibitors of JAK2, JAK3, and STAT3, key proteins in the JAK/STAT pathway, aimed at cancer treatment. We first refined the National Cancer Institute (NCI) database, consisting of 40,000 compounds, using QikProp and SwissADME to select drug-like candidates[2]. The Biotarget Predictor Tool (BPT), developed by our research group and available on the DRUDIT platform[3], was then used in ON/OFF-target mode to predict compounds with high affinity for JAK2, JAK3, and STAT3, while minimizing off-target interactions with TNF-α and p53.

Next, a two-step Docking Virtual Screening Workflow was applied, consisting of Extra Precision (XP) Docking and Induced Fit Docking (IFD), to refine the top candidates. Among them, compound **755435** (Figure 1) exhibited strong binding affinities and stable interactions with JAK2, JAK3, and STAT3, as confirmed by Molecular Dynamics Simulations and Interaction Maps with key active site residues. This multi-target approach, combined with OFF-target minimization, suggests that compound **755435** may offer a dual therapeutic advantage: enhancing efficacy in targeting multiple components of the JAK/STAT pathway while reducing the side effects associated with OFF-target interactions. Our results offer a promising foundation for the further optimization and preclinical evaluation of novel anticancer agents aimed at the JAK/STAT pathway.

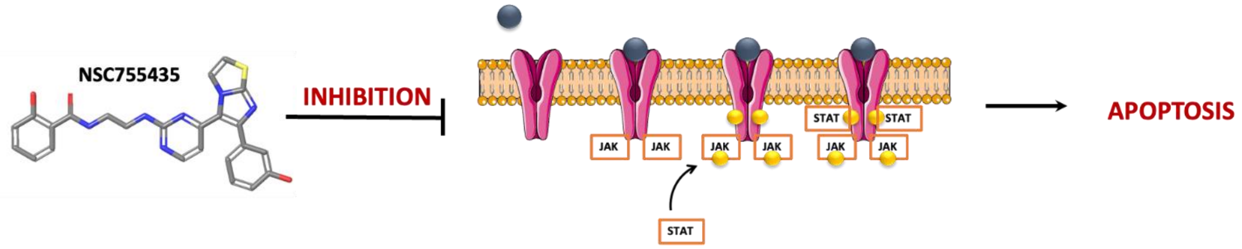

Figure 1. Schematic representation of the JAK/STAT signaling pathway blocked by compound **755435**.

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PO8

On the G4 binding and anticancer effects of copper(II) Schiff base complexes

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Copper, an essential trace element accounting for approximately 100 mg in the average human body, plays a vital role in numerous enzymatic and cellular functions, including cardiovascular health, neuroendocrine activity, and iron metabolism.[1] In contrast to non-essential metals such as platinum, copper is less toxic due to evolved human mechanisms that regulate its levels. Researchers have exploited copper's distinct properties to develop compounds for treating conditions ranging from copper deficiencies to inflammatory diseases. In oncology, several copper(II) complexes are progressing through clinical trials, many demonstrating anticancer effects through the generation of reactive oxygen species and interactions with DNA. Maintaining control over the redox state of the metal is critical for these effects, as exemplified by compounds like $CuPhenCl_2$ (Figure 1).[2] Furthermore, Schiff base copper(II) complexes exhibit strong binding to G-quadruplex DNA (G4)[3]—unique DNA structures implicated in cancer development—which underscores their potential in cancer therapies. Interestingly, CuL^{2+} (Figure 1) has displayed notable catalytic abilities in the oxidation of benzyl alcohols when encapsulated in Zeolite Y.[4] Building on this insight, we hypothesized that CuL^{2+} and related complexes might possess anticancer potential due to their ability to access the +1 oxidation state, thereby potentially inducing ROS production in cancer cells. In this work, we present our latest findings on this family of copper(II) compounds, detailing their G4 stabilization and cytotoxicity against the HepG2 cancer cell line, and demonstrating their in vitro accessibility to the +1 oxidation state.

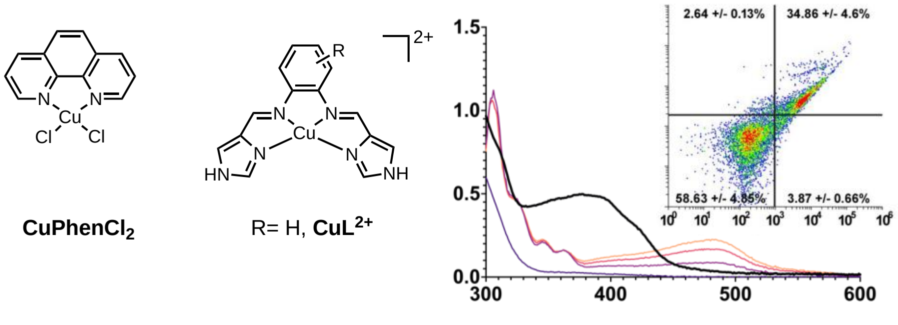

Figure 1. General formula of CuL^{2+} related complexes and examples of studies presented in this work.

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PO9

A literature survey of La^{3+} hydrolysis in aqueous solution.

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Lanthanum, constituting 14.1% of total rare earth elements (REEs), plays a pivotal role in catalytic materials, especially in industrial catalysts. Additionally, lanthanide-based materials have broad applications in cancer treatments, such as biosensing, bioimaging, and photothermal therapy, as well as in waste treatment and various optical, electrical, and magnetic technologies. Lanthanide complexes in metal-organic frameworks (MOFs) are also important for water contaminant removal and the development of chemical sensors. These diverse applications are driven by the distinctive electronic properties of lanthanide (III) centers.The extraction of lanthanum typically involves multiple stages, including mining, beneficiation, and chemical processing, which can be complex and pose environmental challenges, particularly due to the presence of radioactive elements in some ores. To mitigate these issues, recovery of lanthanum from aqueous solutions has emerged as a key strategy for reducing environmental pollution. Understanding the acid-base properties of lanthanum (significantly impact its solubility, coordination chemistry, and interactions with ligands) is essential for comprehending the behavior of La^{3+} in aqueous solutions. However, a review of the literature[1-2] reveals limited and inconsistent data, particularly concerning the characteristics and stability of La^{3+} hydrolytic species. This underscores the need for additional targeted experiments to gain a more comprehensive understanding. For this reason, some experimental data at 298.15K were performed in $NaCl_{(aq)}$ and $NaClO_{4(aq)}$ at different ionic strength I (0.1 to 1 mol dm^{-3}) and at different concentration of La^{3+} (0.5 to 2 mmol dm^{-3}).

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PO10

Development of eco-friendly chromatographic methods to determine oxygen heterocyclic compounds in food and cosmetic products scented with *Citrus*

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Oxygen Heterocyclic Compounds are a group of secondary plant metabolites mainly represented by coumarins (Cs), furocoumarins (FCs) and polymethoxyflavones (PMFs). These molecules are characteristic of *Citrus* fruits, often employed to flavour foods and cosmetics. Unfortunately, these molecules can cause harmful effects by ingestion and following exposure to UVA. So, coumarin content is regulated both in food and cosmetic, while FCs content is regulated only in cosmetic products[1,2,3]. For these reasons, over the years several analytical approaches were applied to determine OHCs in *Citrus* products (GC-FID, HPLC and SFC coupled with UV, fluorimeter, or mass detectors). These methods involve long analysis times or the use of toxic solvents. Therefore, this work focuses on developing rapid analytical methods with minimal environmental impact using chromatographic techniques. The first method developed employing liquid chromatography coupled with a triple quadrupole mass spectrometry detector (HPLC-QqQ-MS). This method allowed to determine 36 target analytes in less than 4 minutes with a consumption of about 3 mL of ethanol per analysis. Quantitative characterization was based on calibration curves built in Multiple Reaction Monitoring (MRM) acquisition mode for each target. Method validation was performed and LoD and LoQ values were less than 1 ppb for most target compounds. So, this method was used to quantify OHCs, contained also at trace levels, in several food and cosmetic samples. However, supercritical fluid chromatography (SFC) has emerged as an innovative analytical technique for analyzing these molecules. Two methods were developed utilizing SFC coupled with a photodiode array detector (PDA) and a QqQ-MS, enabling fast separation with minimal solvent usage in under 8 minutes. Thus, SFC is well-suited for quality control of these compounds in citrus essential oils and finished products.

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PO11

New NHC-Ag and Au-*α*-amino acid complexes as anti-breast cancer agents

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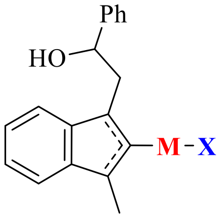
In the last decade, the research on *N*-heterocyclic carbenes (NHCs) complexes with transition metals has attracted scientists' interest for their applications in organometallic catalysis and for their versatile functionalization in medicinal chemistry[1]. Additionally, amino acids represent excellent ligands for transition metals, including silver and gold, although their use in this area remains quite unexplored[2]. Herein, we investigated a new series of Ag(I) and Au(I) complexes, stabilized by NHC ligands and bearing halogen or acetate or carboxylate salts of *tert*-butyloxycarbonyl(Boc)-*N*-protected glycine (Gly), phenylalanine (Phe) or proline (Pro) as anionic ligands (Fig. 1). All the complexes exerted a good anticancer activity against two breast cancer cells, *i.e.* the ER-α positive MCF-7 and the triple negative MDA-MB-231, with IC_{50} values in the low micromolar range. Ongoing studies are directed toward the identification of the target(s) and the mechanism(s) of action underlying the observed anticancer activity.



1	**M**= Ag	**X**= I	**6**	**M**= Au	**X**= Cl
2	**M**= Ag	**X**= OAc	**7**	**M**= Au	**X**= OAc
3	**M**= Ag	**X**= GlyBoc	**8**	**M**= Au	**X**= GlyBoc
4	**M**= Ag	**X**= PheBoc	**9**	**M**= Au	**X**= PheBoc
5	**M**= Ag	**X**= ProBoc	**10**	**M**= Au	**X**= ProBoc

Figure 1. Structures of the studied Ag and Au NHC metal complexes.

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PO12

Eco-friendly Synthesis of Silver and Gold Nanoparticles from *Rumex roseus* Plant Extract and Their Use in Electrochemical Sensing Technologies.

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Metal nanoparticles (NPs) at the nanometer scale, particularly silver (AgNPs) and gold (AuNPs), offer significant advantages in electrochemical applications due to their high surface energy, excellent conductivity, and catalytic properties, which enhance charge transfer at electrode surfaces. Their large effective surface area and electrocatalytic capabilities have made them popular choices as electrode modifiers in the development of electrochemical sensors for electroactive substances.[1,2] In this study, we report the room-temperature synthesis of AgNPs and AuNPs using *Rumex roseus* plant extract as a reducing agent for the first time. The synthesized nanoparticles were characterized by UV-Vis spectroscopy, transmission electron microscopy (TEM), and dynamic light scattering (DLS), confirming their spherical morphology and plasmon resonance. The AgNPs were employed as modifiers of glassy carbon electrodes (GCEs) for the electrochemical detection of hydrogen peroxide (H_2O_2), while AuNPs-modified screen-printed carbon electrodes (SPCEs) were tested for riboflavin (RF) sensing. Further enhancement in sensor performance was observed by using a nanocomposite of AgNPs and reduced graphene oxide (rGO). This study presents a simple and reliable green synthesis route for metal nanoparticles from *Rumex roseus* extract, advancing the development of sensitive electrochemical sensors for H_2O_2 and RF detection.

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Acknowledgements

This work has been partially funded by the European Union (NextGeneration EU) through the MUR-PNRR project SAMOTHRACE (ECS00000022).

PO13

Photostability of newly synthesized 1,4-dihydropyridines: MCR modelling and HPLC analysis

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1,4-Dihydropyridines (DHPs) are well-known for their efficacy as L-type calcium channel blockers, offering significant therapeutic benefits in treating cardiovascular disorders. However, when exposed to light, all DHPs tend to degrade easily, leading to the formation of an oxidation product resulting from the aromatization of the dihydropyridine ring. In this study, the photostability of 19 newly synthesized DHPs was assessed and compared to that of the first-generation DHP drugs. Photodegradation experiments were performed in a light cabinet following the ICH guidelines. Spectrophotometric analysis was employed to monitor the degradation processes, with data analyzed using Multivariate Curve Resolution (MCR) techniques. The modelling results suggest that most of the tested DHPs predominantly formed a pyridine derivative upon degradation. However, for certain compounds, the formation of a secondary photoproduct was also observed. Across all experiments, the lack of fit (LOF) was below 7%, and the explained variance (R^2) exceeded 99.3%, indicating excellent model accuracy. An HPLC-DAD procedure was finally performed to confirm the number of the photoproducts and their absorbance spectra. Chromatographic conditions were optimized to achieve clear resolution of closely eluting species. Our findings indicate that certain structural modifications in DHPs improve their photostability, offering insights into the design of more stable DHP-based drugs. These improvements could lead to better pharmacokinetic properties and expanded clinical applications.

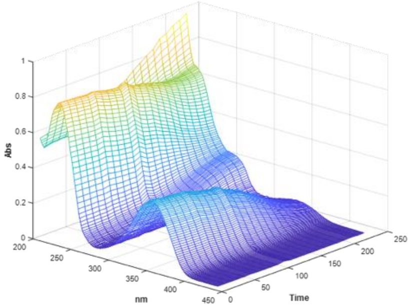

Figure 1. Photodegradation experiment of a DHP. Spectral sequences

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PO14

The impact of chalcogen-chalcogen bond formation in New Delhi metallo-β-lactamase 1 enzyme to contrast antibiotic resistance

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The enzyme known as New Delhi metallo-β-lactamase 1 (NDM-1)[1] contributes to the drug resistance of numerous bacteria to the majority of commonly used antibiotics, including carbapenems, cephalosporins, and penicillins[2]. In order to overcome this bacterial defense mechanism and restore the efficacy of antibiotics, blocking NDM-1 is rapidly attracting a lot of attention. Ebselen (EbSe), one of the inhibitors most recently tested against the enzyme,[3] demonstrated encouraging outcomes. EbSe, well known for its many health benefits, uses its selenium atom to target the NDM-1 active site at Cys208 promoting the formation of covalent bond (Se_{EbSe}-S_{Cys208}) the release of catalytic zinc ion from the active pocket. Since little is known about the inhibitory mechanism of EbSe, it would be very beneficial to learn more about it. The inhibition mechanism of NDM-1 with EbSe is investigated using calculations based on density functional theory, then µs-long molecular dynamics simulations provide further insights on the structural consequences of the inhibition. To examine the many mechanistic pathways for the covalent bond (Se_{EbSe}-S_{Cys208}) formation, a sizable model of the NDM-1 active site is constructed. Elucidation on the role of Lys211 during the inhibition mechanism is also provided by mutation *in silico*. Ebsulfur (EbS) molecule is also examined aimed to compare its behavior with that of the relative selenium. In addition to demonstrate the involvement of the L3 and L10 loops in the inhibition, unbiased and biased (Umbrella sampling) molecular dynamics simulations are further performed to investigate the expulsion of Zn cation from the active site.

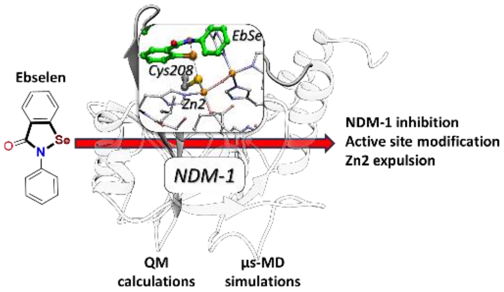

Figure 1 *Scheme of the covalent bond effect promoted by Ebselen on NDM-1.*

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PO15

Design, synthesis and biological evaluation of dipeptide nitriles as inhibitors of rhodesain of *Trypanosoma brucei rhodesiense*

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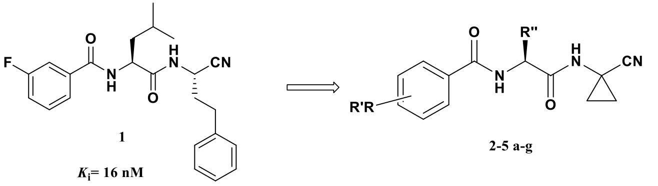
Human African Trypanosomiasis (HAT) belongs to the Neglected Tropical Diseases (NTDs) and is widespread in Africa, because of the poor living conditions[1]. HAT, also known also as sleeping sickness, is caused by a protozoan of *Trypanosoma* genus. *Trypanosoma brucei gambiense* is responsible for a chronic form of the disease, while *Trypanosoma brucei rhodesiense* is able to induce the acute form of HAT. Pharmacological treatment of HAT is limited to the use of dated drugs with problems related to toxicity, route of administration and limited spectrum of action. For this reason, there is an urgent need to find new targets for HAT treatment. Rhodesain, a cysteine protease of *Trypanosoma brucei rhodesiense*, could be considered a promising target for the development of new antitrypanosomal drugs, because of its key role in the life cycle of the parasite[2]. In recent years, our research group has been focused on the design, synthesis and biological evaluation of novel rhodesain inhibitors for HAT treatment starting from the reversible rhodesain inhibitor **1**[3], we now developed a new series of dipeptide nitriles **2-5 a-g**. (Figure 1). The new inhibitors differ from the lead compound **1** because of the presence of a cyclopropyl carbonitrile instead of a homophenylalanine bearing a nitrile as warhead; this modification has been made because a cyclopropyl carbonitrile is present in the macrolactam with whom rhodesain has been co-crystallized. At the P2 site, a leucine, a phenylalanine, a cyclohexyl alanine or a cyclopropyl residue were introduced to investigate the impact on rhodesain inhibition. The amino group of these residues was protected with fluoro-benzoyl substituents spanning into the S3 pocket, due to the high binding affinity towards rhodesain of the fluorinated lead compound **1**. All the new synthesized inhibitors were tested in fluorimetric assays against recombinant rhodesain and they were proven to inhibit the trypanosomal cysteine protease in a reversible manner and with K_i values in the nanomolar range.



1

K_i = 16 nM

2-5 a-g

RR'= H, 2-F, 3-F, 4-F, 2,4-diF, 2,6-diF, 2,5-diF, 3,5-diF
R''= CH_2-$CH(CH_3)_2$, -CH_2Ph, Cp, CH_2-Cy

Figure 1. Structure of the lead compound **1** and of novel rhodesain inhibitors **2-5 a-g**

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PO16

Multifaceted derivatives of chrysin: evaluation of their vasorelaxant, antioxidant and antiinflammatory properties to face hypertension

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Hypertension is a multifactorial disease that affects nearly one billion adults each year and is espected to increase by 25% higher by 2025[1]. One of the main mechanisms involved in the pathogenesis of this disease is endothelial dysfunction, characterized by vasoconstriction, leukocytes adhesion, reduced nitric oxide production and, consequently, increased in vascular tone with loss of elasticity of the aorta and the other large arteries. At the endothelial level ionic channels play an important role, particularly, calcium and potassium channels. Alterations in vascular and cardiac $Ca_V1.2$ calcium channel activity have been associated with hypertension[2]. Various clinical studies have also demonstrated the strong correlation between high blood pressure values and the increase of “inflammasome” players such as C-reactive protein or cytokines, ROS etc the presence which correlates with the risk of developing cardiovascular complications and thus hypertension[3]. Regular consumption of polyphenol-rich foods has been shown to be inversely related with cardiovascular morbidity and mortality. In this work, chrysin, a flavone that can act as $Ca_V1.2$ channel inhibitor, was selected as the lead compound, to create a library of challenging derivatives. The compounds were synthesized and evaluated for their *in vitro* vasoactivity by electrophysiological experiments on denuded aortic rings but also for their in vitro antioxidant and anti-inflammatory activity, first by colourimetric assays (ABTS and DPPH) and then on RAW 264.7 cells. All the compounds showed a vasorelaxant profile comparable to the parent compound but two derivatives, Chrys-NO_2 and Chrys-NH_2 significantly antagonised both high KCl-induced contraction and $I_{Ba1.2}$ in rat tail artery preparations. Chrys-NO_2 also gave back promising results in the Griess assay, being very active at a concentration of around 10 µM and showing much better activity than that exhibited by the parent compound but also than indomethacin, with no toxic effects on normal cells. Taken together these data demonstrate how small chemical modifications can alter the pharmacological effects of polyphenols. Above all, compounds that can counteract different mechanisms involved in the disease are promising starting points for the development of antihypertensive drugs

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PO17

Discovery of a Potent Natural HDAC8 Inhibitor: Virtual Screening and In Vitro Validation

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HDAC8 plays a crucial role in regulating chromatin structure and gene expression through histone deacetylation, and its deregulation has been associated with various diseases, including cancer.[1] In this study, we conducted an *in silico* screening to identify potential HDAC8 inhibitors. We analysed 11 crystal structures of HDAC8 and selected those complexed with the five ligands exhibiting the greatest variation in chemical structure as templates for a shape-based virtual screening. This effective method identifies small molecules that resemble the shape and function of a reference ligand and was applied to a dataset of 307814 natural compounds derived from the ZINC database.[2] The top 9737 compounds were docked using the Glide SP protocol[3], and subsequent MM-GBSA calculations led to the identification of 40 compounds with favourable binding free energies. After clustering, 13 representative compounds were selected for further evaluation.

Among the eight commercially available compounds tested *in vitro* using a fluorometric HDAC8 inhibition assay, five exhibited low inhibition activity. Notably, the best hit demonstrated a remarkable inhibition rate of 97.56% at 1 μM, outperforming the reference inhibitor trichostatin A (TSA), which showed 91.09% inhibition at 10 μM. Binding mode analysis revealed that this compound forms multiple stabilizing interactions within the enzyme's active site, including π-π interactions and hydrogen bonds. To gain deeper insights into these interactions, molecular dynamics simulations are currently ongoing to evaluate the stability of the complex and its behaviour over time.

Proliferation assays are also underway on several cancer cell lines, including MD-MAB157, MCF-7, Caco-2, HeLa, K1, as well as Nthy-ori-3-1 which is a non-tumour cell line so as to assess the compound's selectivity.

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PO18

Hydrogen production by photoreforming using different TiO_2 or Nb_2O_5 composites with graphene or graphene oxide as photocatalysts.

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The photoreforming of aqueous solutions containing organic compounds combines the photocatalytic splitting of water with the oxidation of organics in a single process under ambient conditions. TiO_2 and Nb_2O_5 suffer from limited absorption of sunlight due to their large bandgap (~3 eV) and low photocatalytic activity due to the rapid recombination of charge carriers. Various strategies have been employed to solve these problems, and the combination of TiO_2 nanoparticles (NPs) with carbon nanomaterials, such as carbon nanotubes, graphite oxide (**GO**) and graphene (**G**), has been proposed as a suitable method to increase photocatalytic activity. From previous work, we have seen that home-made Nb_2O_5 [1] from ANbO (**A**mmonium **N**io**b**ium **O**xalate) is an excellent catalyst that has activity comparable to that of TiO_2.

This research focuses on the development of hetero-junctions synthesized with different weight ratios between carbon materials (5, 10 or 20 %) and TiO_2 (named Ti-G 10:X or Ti-GO 10:X, where X represent the mass of G or GO per 10 g of TiO_2) or Nb_2O_5 (named Nb-G 10:X or Nb-GO 10:X, where X represent the mass of G or GO per 10 g of Nb_2O_5) for the photo-reforming of organics dissolved in water [2]. In these composites, the oxide semiconductor acts as the photocatalyst, while the carbon materials (commercial or homemade) act as a reservoir and electron carrier, facilitating the transfer of electrons to the reaction sites. Photoreforming tests of water solutions of ethanol or glycerol or water dispersion of microplastics were conducted both under UV and natural sunlight irradiation. The activity of the catalysts was compared based on the amount of hydrogen produced. The catalysts were tested without and with the use of platinum as co-catalyst. In the first case, small amounts of hydrogen were obtained. The best result was obtained in the presence of Ti-G 10:1 with 1wt% of Pt reaching a productivity of 311 $mmol \cdot h^{-1} \cdot g^{-1}$ (AQE of 100 %) under UV light and 13 $mmol \cdot h^{-1} \cdot g^{-1}$ under natural sunlight.

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PO19

Cyclopropane derivatives with antiviral activity acting on Sigma-1 Receptor

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Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2), belonging to the coronavirus family, is the aetiological agent of the COVID-19 pandemic. Despite ongoing research, there remains an urgent need for effective treatments. Consequently, novel therapeutic targets involved in the pathogenesis of COVID-19 have been explored, with particular attention given to the Sigma-1 receptor (σ1R) due to its pivotal role in cellular stress responses during viral infections.[1]

Notably, the σ1R is closely linked to SARS-CoV-2 replication, and its inhibition has significantly reduced viral load. Furthermore, research has demonstrated that ligands targeting σ1R can provide mitochondrial protection, alleviate cellular stress, and safeguard vital organs such as the heart and lungs, thereby mitigating long-term damage and reducing mortality risk.

Building on this promising avenue, cyclopropane derivatives have been designed and successfully synthesized as potential σ1R ligands, offering a novel approach to combat COVID-19.[2]

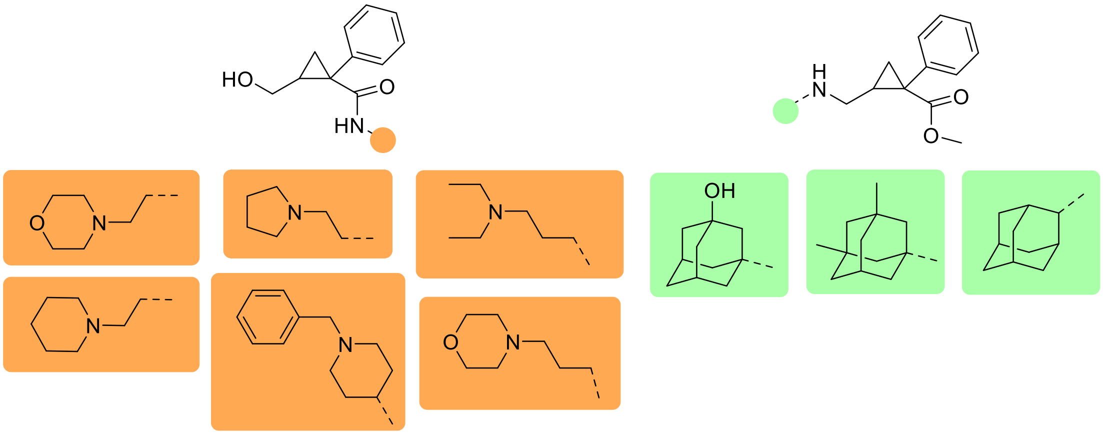

Figure 1. Structures of synthesized compounds.

ADMET prediction studies have been carried out on the synthesized compounds using the free web tools SwissADMET and DataWarrior software. Docking and molecular dynamics studies are currently underway. Binding assays will be conducted to assess the affinity *versus* σ1R.

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PO20

Eco-Sustainable SERS sensors for Cultural Heritage applications: achievements and future developments (SAMOTRACE project)

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As part of the SAMOTRACE project, IPCF Messina is developing an innovative approach for fabricating flexible SERS (Surface-Enhanced Raman Spectroscopy) sensors based on cellulose substrates (reclaimed from recycled and ecological paper) decorated with nanostructured Ag thin films produced by pulsed laser deposition. A wide range of paper samples was tested, as morphology and texture can play a significant role in SERS efficiency (Figure 1). After characterizing the deposited substrates using UV-Vis absorption spectroscopy, SEM microscopy, and surface profilometry, the SERS activity was evaluated by detecting the probe molecule (Rhodamine 6G) in solutions drop-cast onto the sensors, with concentrations ranging from 10^{-2} M to 10^{-10} M. Measurements were conducted using a handheld Raman spectrometer with dual excitation laser lines at 785 nm and 833 nm. A detection limit as low as 10^{-10} M was observed across all tested paper types with R6G. To achieve a fully eco-friendly and sustainable process, we are currently exploring the use of alternative, natural and non-toxic dyes extracted from bacterial sources as probe molecules. Additionally, we are testing new methods to produce Ag nanoparticles using a chemical approach (colloidal Ag). These materials not only demonstrate good sensing performance but also aim to reduce environmental impact through renewable sourcing and a fully green manufacturing process.

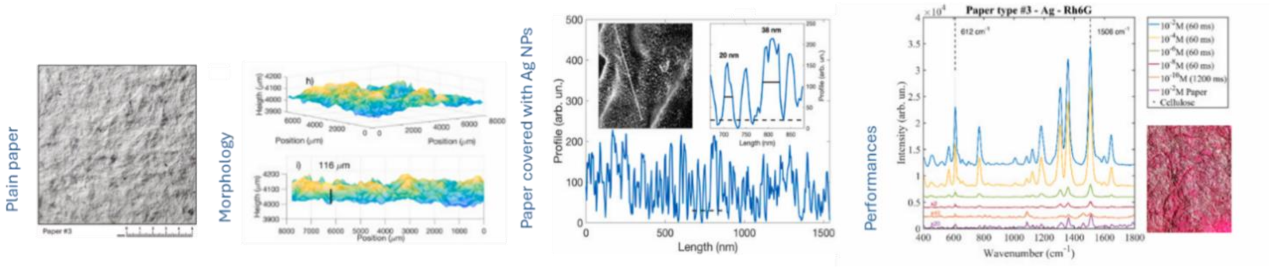

Figure 1. Performance of the SERS sensors with Rhodamine 6G.

This work has been funded by NextGeneration EU, through the MUR-PNRR project SAMOTHRACE (ECS00000022).

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PO21

Assessing the hydrolysis of Gd(III) in aqueous NaCl and $NaNO_3$ solutions coupling potentiometry and light scattering

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The relevance of assessing the chemical speciation of metal cations, particularly those belonging to the list of the *Critical Raw Materials* in aqueous solutions is nowadays much more important than ever, especially considering that the consumption of metals as a feedstock for the information and communication technology industry is largely increasing as well as the need of re-cycle such metals from e-waste. In this context, the modelling of the metal cation hydrolysis constants and solubility product is a cornerstone to plan sustainable recovery routes. In this contribution, a study on the hydrolysis and solubility of gadolinium(III) is reported. A preliminary literature analysis evidenced the presence of five hydrolytic species with various stoichiometry, namely $Gd(OH)^{2+}$, $Gd(OH)_2^{+}$ $Gd(OH)_{3(aq)}$ for the mononuclears, $Gd_2(OH)_2^{4+}$ and $Gd_3(OH)_4^{5+}$ as the polynuclear ones[1]. By analysing the collected data, reported at different ionic strength, temperature and ionic media, it was possible to understand that only for the first hydrolysis constant, $Gd(OH)^{2+}$, published data are sufficient to allow for a robust data analysis, whereas the stability of other species is still far from being established. The reason of this lack of information, which is common to many other metal cations, rely on the fact that the precipitation of the insoluble $Gd(OH)_{3(s)}$ species starts immediately after the formation of the aqueous $Gd(OH)^{2+}$ and, especially, $Gd(OH)_2^{+}$ and $Gd(OH)_{3(aq)}$ ones. Preliminary classical potentiometric titrations confirmed that it is very difficult to accurately detect the precipitation pH of the $Gd(OH)_{3(s)}$ species. Therefore, a dedicated experimental setup has been established coupling potentiometry and UV-vis spectrophotometry. In particular, aqueous solutions containing Gd^{3+} ($0.5 \leq c_{Gd(III)}$/mmol dm$^{-3} \leq 20$) and a supporting electrolyte (NaCl or $NaNO_3$) is titrated with standard sodium hydroxide solutions in a thermostatted vessel (± 0.1 K) between pH ~ 3 and pH ~ 7. After each addition of the alkali solution the pH is measured by means of an ISE-H^+ electrode and the light scattering (LS) is measured through an optic probe working only as a detector and with the optic path placed orthogonally to an external white light source in a dark environment. When small particles, such as those of amorphous $Gd(OH)_{3(s)}$, are formed the signal read by the detector increases significantly and the solution pH is recorded. The linearity of the LS response was tested with Gd_2O_3 nanoparticles. Moreover, the intensity of the scattered light is read as a function of time within two different NaOH additions to monitor the kinetic profile of such phenomenon.

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PO22

Decomposition Mechanism of Isoeugenol on a Pt_{10} Cluster: A DFT Investigation Followed by Microkinetic Analysis

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In a scenario of declining fossil resources and severe environmental concerns related to their use, biomass valorization emerges as a promising solution to meet the global demand for sustainable and renewable alternatives. Lignin, the most thermally stable component of biomass, is unique in its potential to provide aromatic-based compounds and the selective transformation of lignocellulosic biomass into value-added fuels has gained increasing interest. Although pyrolysis is a well-studied method for converting lignin into liquid fuels (bio-oils), it often leads to a variable and unpredictable range of products that complicates separation and increases costs. In this respect, heterogeneous catalysis plays a crucial role in enhancing the viability of biomass conversion by ruling product selectivity, even if the removal of oxygenated groups remains a significant challenge. Quantum chemistry has become an essential component of catalysis research. Density Functional Theory (DFT) in particular serves as a powerful tool for investigating catalytic processes and understanding their fundamental steps and mechanisms at the atomic scale.

The present investigation was oriented towards the computational mechanistic analysis of the isoeugenol catalytic decomposition on a subnanometric platinum cluster. Showing a number of functional groups typical of the chemicals of biomass origin, isoeugenol is considered a well representative experimental and computational model. A ten-atoms platinum cluster was selected as a subnanometric catalytic system, being Pt a computational reference element for hydrogenation reactions. The study is indeed framed in a broader project that aims at exploring potential reactions of isoeugenol also in presence of H_2, namely hydrodeoxygenation routes. The reported computational study outlines the energy barriers and the intermediates involved in the conversion of isoeugenol to benzene derivatives, through removal of the oxygenated groups and saturation of the propylenic chain. A microkinetic analysis (Simplified Christiansen Method) was conducted, utilizing detailed DFT energetics of all the studied mechanisms, which provided unbiased estimates of the kinetic constants at specific temperatures and allowed to identify the fastest reaction pathways.

PO23

Design and synthesis of nanocarbon-based hybrid materials for pollutants removal and degradation

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Human activities and industrial effluents introduce a variety of contaminants into water resources, such as dyes, pharmaceutical waste, pesticides and heavy metals. Conventional water treatment technologies could not effectively remove some of waste. Carbon-based nanomaterials have shown substantial potential in the removal of pollutants due to their large chemically active surface, high electrical conductivity, and high chemical stability[1]. In particular, carbon nanotubes (CNTs) can be used as support material for the dispersion of metal oxide and semiconductor nanoparticles (NPs)[2]. Our goal is to synthetize a series of hybrid materials based on properly functionalized multi-walled carbon nanotubes (MWCNT) used as support for co-immobilization of ZnO and silver nanoparticles. We have started to investigate the effect of the immobilization of metal oxides onto MWCNTs functionalized with a polyamine network obtained after the reduction of a bis-vinylimidazolium salt precursor, which was polymerized onto the surface of pristine MWCNTs. Preliminary results on the photocatalytic activity of all materials toward toluidine blue degradation are presented.

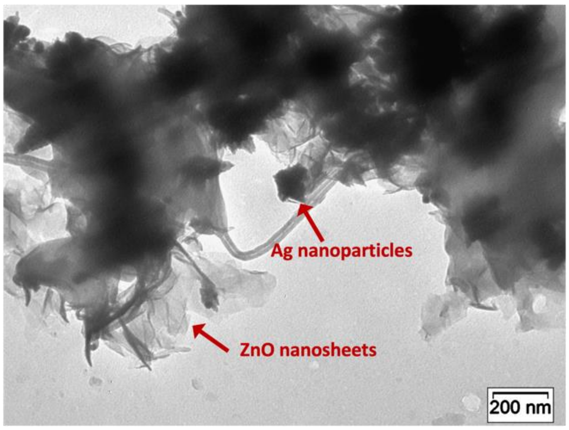

Figure 1: TEM image of MWCNT-polyamine-ZnO/Ag.

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PO24

Sequestration of metal and organometal cations using a natural occurring polyphenol

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Metal and organometal cations are dangerous pollutants of natural waters, causing severe environmental and biological problems[1,2]. In contrast, gallic acid (*GA*) is a naturally occurring polyphenol found in citrus fruit peels, honey, grapes, hops, oak bark, and tea leaves[3], displaying several beneficial properties[4]. Performing a contaminant speciation study in conditions simulating the ones characteristic of real environmental matrices, is essential for gaining information on the pollutant mobility, transport, toxicity, environmental impact and fate.

In this light, this contribution reports the results of an investigation on the *GA* stability, acid-base properties and interactions with cadmium(II) (Cd^{2+}) and two organometal cations, namely methylmercury(II) (CH_3Hg^+) and dimethyltin(IV) ($(CH_3)_2Sn^{2+}$). The experimental measurements were carried out by means of potentiometry, UV-Vis spectrophotometry, spectrofluorimetry and ^{1}H NMR spectroscopy at different temperatures ($288.15 \leq T/\mathrm{K} \leq 318.15$) and ionic strengths ($0.10 \leq I/\mathrm{mol\ dm^{-3}} \leq 1.00$) in NaCl ionic medium, the principal inorganic constituent of many natural fluids[5]. The thermodynamic data showed for gallic acid higher complexing ($\log K_{pqr}$) and sequestering ($pL_{0.5}$)[6] abilities, as well as metal affinity (pM)[7], towards $(CH_3)_2Sn^{2+}$ with respect to CH_3Hg^+ and Cd^{2+}, demonstrating the ligand promising and selective performances as potential decontaminating agent for the dimethyltin(IV) remediation from polluted sites. This study could also contribute to the development of environmental strategies aimed at the production of new gallic-acid based sustainable materials dealing with the metal and organometal contamination issue, as well as for potential applications in various industrial fields.

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PO25

Novel piperazinyl-quinoline molecular hybrids with anticancer activity: synthesis, in silico insights and in vitro evaluation on NCI cancer cell lines

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Molecular hybridization, i.e. the integration of known bioactive structural components into a single chemical entity, is one of the most interesting strategies in medicinal chemistry to afford hybrid molecules with enhanced biological activity.[1] In the field of anticancer research, quinoline and piperazine stand out among the most promising and recurring pharmacophoric moieties, being the central cores of many drugs approved in therapy.[2-4] Against this background, a new series of 4-(4-benzoylpiperazin-1-yl)-6-nitroquinoline-3-carbonitrile hybrid compounds (**1a-l**) with potential anticancer activity is presented.

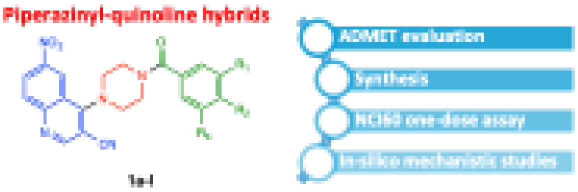

Figure 1. General chemical structure of the 4-(4-benzoylpiperazin-1-yl)-6-nitroquinoline-3-carbonitrile hybrids **1a-l** investigated.

The designed compounds were first evaluated in silico to determine their ADMET properties and drug-likeness profiles and then successfully synthesized using appropriate multistep preparative procedures. Preliminary in vitro biological screening was performed by the National Cancer Institute under the DTP-NCI60 program. The entire series of piperazinyl-quinoline compounds showed interesting anticancer activity, particularly against the UO-31 cell line of renal cell carcinoma (RCC). Induced fit docking (IFD) and molecular dynamics (MD) simulations offered deeper insights into the potential mechanisms of action, suggesting that the compounds **1a-l** could robustly interact with key oncogenic proteins involved in cancer development, including RCC. These encouraging in vitro and in silico results provide a solid foundation for further investigation and lead optimization processes.

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PO26

Design and synthesis of a magnetic nanomaterial based on halloysite for potential theranostic application

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Nowadays, finding systems capable to simultaneous treat and diagnose various diseases, thus acting as theranostic materials, is a challenging.[1] Regarding the diagnostic aspect, fluorescent pH probes have attracted increasing interest for monitoring pH variations inside biological systems.[2] However, most of the commonly used chromophores are hydrophobic and therefore their use in the biological field is limited. To overcome this problem, several carrier systems, such as halloysite nanotubes (HNTs), are often employed for application in bioimaging, Indeed, HNTs increases the chromophore solubility in physiological conditions and boost the fluorescent properties.[3] In addition, compared to other nanoparticles, halloysite is naturally occurring, eco and bio-compatible.

Regarding the therapeutic aspect, ferroferric oxide nanoparticles (Fe_3O_4NPs) can be exploit for their chemodynamic activity for cancer treatment *via* Fenton or Fenton-like reaction thanks to the production of highly toxic hydroxyl radicals (·OH).[4]

Herein we report two different approaches for the covalent modification of HNTs external surface with an halochromic switch to develop a biological probe. The obtained nanomaterial was characterized by different physical-chemical techniques, its morphology was examined by TEM and the photophysical properties were investigated both in dispersion and solid state. This nanomaterial was used as scaffold for the immobilization of Fe_3O_4NPs by the co-precipitation method and the chemodynamic activity was tested in the oxidation of TMB as chemical probe.

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PO27

Inhibition of HO-1 by Bioisosteric Replacement of the Amide Function

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Heme oxygenase 1 (HO-1) is an inducible cytoprotective enzyme responsible for the regio-selective catabolism of heme. High levels of HO-1, in some types of tumors, has been demonstrated to induce the formation of a prometastatic tumour microenvironment that favors immunosuppression, angiogenesis and the induction of chemoresistance phenomena. [1] Hence, HO-1 inhibition, as a stand-alone or as adjuvant agent during chemotherapy, is gaining more and more interest as an innovative pharmacological approach. We recently reported on new HO inhibitors based on a *N*-methylacetamide scaffold (Figure 1). [2] However, ADME preliminary studies showed half-life issues for this class of compounds. Bioisosterism approach, has been applied to this class of compounds in order to modulate metabolism, and enhance biological properties of the lead compound. *In vitro* HO-1 inhibition studies showed, for some derivatives, IC_{50} values below 0.1 μM. Obtained results suggested that the biosisosteric strategy was successful in identifying new potent HO-1 inhibitors.

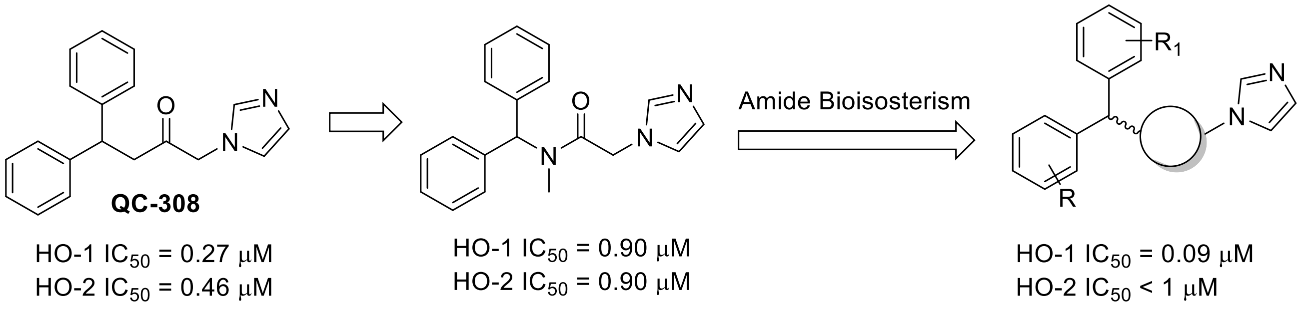

Figure 1. Bioisosteric replacement of the amide function.

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PO28

Prediction of Activity and Selectivity Profiles of Sigma Receptor Ligands Using Machine Learning Approaches

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Sigma receptors (SRs) are emerging as important therapeutic targets due to their involvement in various biological pathways. They are divided into two subtypes: Sigma 1 Receptor (S1R), primarily distributed in the central nervous system and related to neuroprotection and neurodegenerative diseases, and Sigma 2 Receptor (S2R), mainly expressed in cancer cells and associated with cell proliferation and apoptosis.[1,2] Despite structural differences, both receptors share similar binding site features and ligand recognition, which underscores the importance of identifying selective ligands for therapeutic design.[2] In this project, we developed three distinct machine learning (ML) approaches based on classification, regression, and multiclass models to predict both the activity and selectivity of SRs (Figure 1). To achieve this, we trained a series of ML models on high-confidence data sourced from various public databases and in-house data. The datasets were systematically organized and processed for each of the three workflows. For the classification, regression, and multiclass models, we employed algorithms such as Random Forest, Support Vector Machine, and Gradient Boosting, using molecular descriptors and chemical fingerprints to represent the compounds' properties. Rigorous hyperparameter tuning and model validation were performed using Nested Cross-Validation to ensure robust and accurate predictions. These ML-driven approaches offer a powerful tool for identifying selective compounds, with the potential to accelerate the discovery of novel, potent, and selective ligands for S1R and S2R.

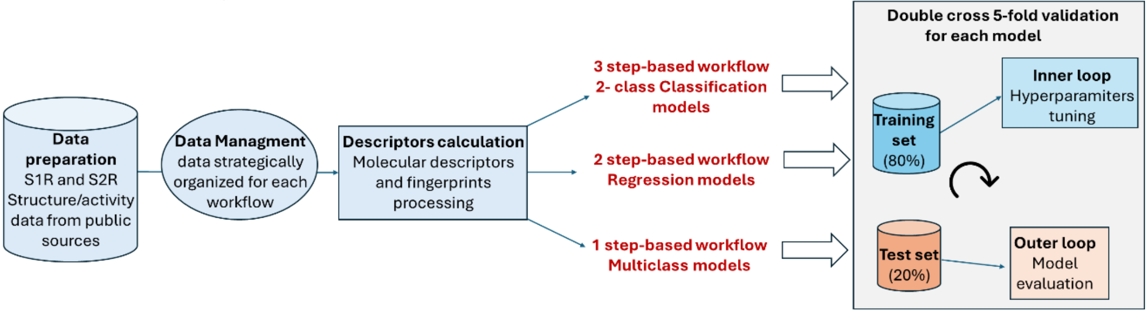

Figure 2. Graphical flow chart of the three ML-based approaches.

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PO29

Is It Possible to Fight Climate Change? Maybe! Let's Start Teaching the Environmental Respect.

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Climate change refers to the long-term increase in temperature, precipitation, and other atmospheric conditions on Earth. This phenomenon is it is mainly due to human activities, especially the burning of fossil fuels such as coal, oil, and natural gas, which release greenhouse gases (GHGs) like carbon dioxide (CO_2) into the atmosphere. These gases trap heat, leading to the warming of the planet, a process known as the greenhouse effect.

One of the most visible effects of climate change is global warming, with average temperatures increasing significantly over the past century. This warming has led to melting glaciers, rising sea levels, and more extreme weather patterns. For instance, hurricanes, droughts, and wildfires are becoming more frequent and severe due to the changing climate, impacting ecosystems and human communities alike. The effects of climate change are not uniform; they vary by region and have complex implications for biodiversity, agriculture, water resources, and human health. Many species are struggling to adapt to the rapidly changing conditions, leading to shifts in migration patterns and, in some cases, extinction. For agriculture, unpredictable weather patterns threaten crop yields and food security, potentially leading to economic challenges and hunger.

Efforts to mitigate climate change focus on reducing greenhouse gas emissions and transitioning to renewable energy sources, such as wind, solar, and hydroelectric power. Additionally, protecting forests and increasing green spaces can help absorb CO_2 from the atmosphere.

Despite these efforts, adapting to the current and future impacts of climate change remains a critical challenge.

The "Digital Green Project" (Erasmus+KA220; *2022-1-TR01- KA220-SCH-000087638*) wants to educate about environmental protection to fight climate change, promoting resilience and encouraging sustainable practices in the energy, agriculture and urban planning sectors, which are essential strategies to minimize negative effects on both the environment and human societies.

Turkey, Germany, Czech Republic, Italy: 4 nations, 6 partners engaged in a two-year project which involves the exchange of professors and students to disseminate good practices aimed at respecting the environment.

PO30

Photocatalytic glyphosate degradation in a combined process with microalgal biologic treatment

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The rapid population increase has driven a surge in food demand, leading to intensive agricultural practices so the use of herbicides in agriculture has grown and glyphosate is one of the most widely employed[1]. Its excessive use has raised concerns about its potential impacts, being classified as a likely human carcinogen[2]. Heterogeneous photocatalysis is an effective technology for treating wastewater in order to oxidise persistent pollutants and TiO$_2$ has been identified as one of the best photocatalysts[3]. The photocatalytic degradation of pollutants before the mineralization can give rise to chemical intermediates that are also toxic and cannot be released in groundwaters. In this study, photocatalysis and microalgae treatments were combined in photobioreactors to study the glyphosate degradation. The aim of the work is combining both processes for the complete mineralization of the pollutant in a two stage process, i.e. the photocatalytic degradation of glyphosate in the presence of commercial Evonik P25 TiO$_2$ would lead to the formation of products such as glycine, phosphate, nitrate, ammonium, along with acetic, oxalic and formic acids that are nutrients for microalgae, that represent an emerging and efficient microorganism for wastewater biologic treatment[4]. Coupling the photocatalysis with a biological microalgae-based treatment, in a two-step process, enhances the mineralization efficiency, achieving removal global efficiencies higher than with the single separated processes. This study, hence, demonstrates that photocatalysis and microalgae combined treatment is an eco-friendly method for the treatment of glyphosate-polluted wastewater. Figure 1 represents the evolution of glyphosate and some of its products during the irradiation under UV in the presence of P25 and the microalgae grow in the solution after the photocatalytic process.

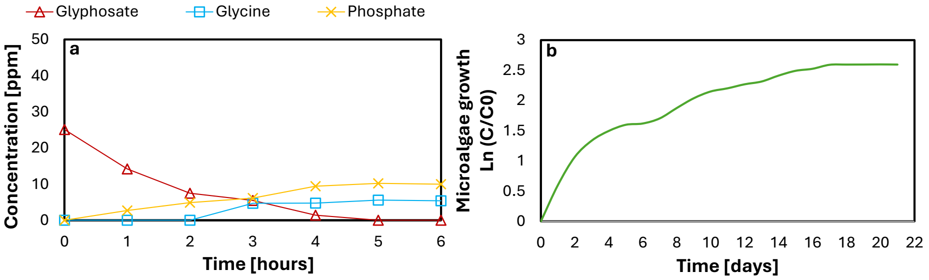

Figure 1. (a) Glyphosate, Glycine and Phosphate trend during the photocatalytic treatment; (b) Microalgae growth in the solution obtained after photocatalysis.

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PO31

Search for new antifouling materials based on structurally optimized quaternary ammonium salts

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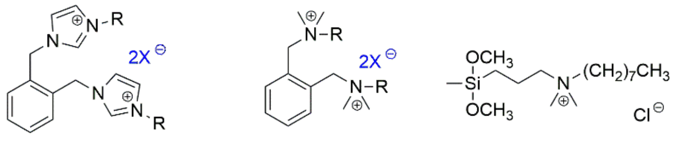
In the marine environment, micro- and macro-organisms can colonize the surface of ship hulls or platforms, resulting in increased erosion and fuel consumption, reduced ship manoeuvrability and environmental impact.[1] New approaches to blocking the formation of biofilms appear to be the most promising in the materials science community. Particularly, non-fouling or fouling-releasing approaches are more favoured than biocide-releasing approaches due to their greater environmental sustainability and durability. Quaternary ammonium salts (QASs) are commonly used to design contact-kill surfaces with non-leaching biocidal motifs.[2] Here, a library of quaternary aliphatic and aromatic ammonium compounds, including QAS-based silanes, was synthesized. The structure-activity relationship was studied by evaluating the antibacterial activity against a Gram-negative strain highly resistant to environmental stimuli.

Hydrophobic ionic liquids with general structures **1** and **2** could have applications as antibacterial additives for oil-based in super-repellent and contact-killing slippery liquid-infused porous surfaces (SLIPS).[3] In the meantime, cross-linked polydimethylsiloxanes and silica materials, that can prevent the formation of microbial biofilms, have been developed using the antibacterial silane **3**. As a preliminary test, the functionalized silicas were added to commercial antifouling paints to study their behaviour when immersed in seawater.



1 **2** **3**

X= Docusate anion; R= Alkyl chain

Figure 1. Hydrophobic ionic liquids (**1** and **2**) and QAS-based silane (**3**) as candidates for designing antifouling materials

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PO32

Incorporation of a supramolecular copolymer in a new water-dispersible microemulsion for drug delivery systems

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Polymeric nanoparticles[1] have attracted a great deal of attention in nanomedical applications over inorganic nanoparticles due to their higher biocompatibility and biodegradability. Supramolecular polymers[2] are macromolecular assemblies composed of monomeric units held together by non-covalent and reversible interactions that can be successfully used in the design of stimuli-responsive nanoparticles. We have recently reported the AA/BB-type supramolecular polymerization of a bis-pillar[5]arene dicarboxylic acid monomer (**H**) in the presence of a mixture of complementary bis-guests alkylidene- and perylene-bisimide-bis-imidazole (**G1** and **G2**, respectively).[3] It has been shown that the supramolecular copolymer **H**/**G1**/**G2** retains the properties of the parent bi-component systems, that is, **H**/**G1** solubility and **H**/**G2** photoresponsiveness; thus the assembled or disassembled state of the copolymer can be revealed by a change in luminescence due to the complexation/decomplexation of **G2** in the pillararene cavities. Herein we report the formation and analysis of nanoparticles produced by the incorporation of **H**/**G1** and **H**/**G1**/**G2** polymers into water-dispersible CTAB (cetyltrimethylammonium bromide) and their potential applications in the biomedical field.

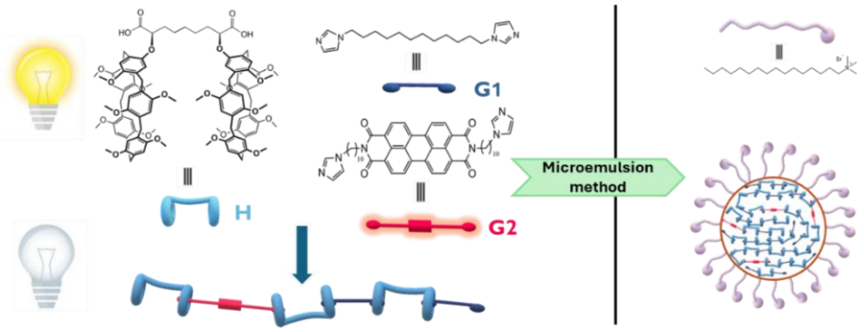

Figure 1. Illustration of the **H**/**G1**/**G2** supramolecular copolymer and its nanoparticles.

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PO33

Design, synthesis and *in vitro* evaluation of 4-(1-piperazinyl)phenol-containing BODIPY targeting Tyrosinase

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Tyrosinase (TYR, EC 1.14.18.1) is the regulatory metallo-enzyme involved in the biosynthesis of melanin pigment. TYR possesses a strongly conserved bicopper active site and catalyzes the oxidative chemical conversion of Tyrosine and/or L-Dopa to melanin. Given that the abnormal TYR activity in melanocytes is responsible for different skin hyper-pigmentation disorders and melanoma, it has been argued that TYR could represent a nice biomarker for these pathologies. Therefore, the inhibition and the high sensitivity detection of this protein is of great relevance, not only in therapeutic treatment but also for observing its activities in biological processes and, thus, for its significance in clinical diagnosis.[1] We have previously reported that the 4-(1-piperazinyl)phenol and several 4-(1-piperazinyl)phenol-based compounds were very potent inhibitors of *Agaricus bisporus* (AbTYR) and human tyrosinases (hTYR).[2,3] As a continuation of these studies, we designed a small series of chimeric molecules as potential TYR biomarker by combining the 4-(1-piperazinyl)phenol pharmacophoric moiety and the BODIPY dies as fluorescent probes. To investigate the optimal distance between these two fundamental features, a three-carbon atom chain or an aromatic ring acted as bridge feature. Each obtained compound was spectrophotometrically tested against AbTYR and the hypothetical binding mode was predicted by docking simulations (Figure 1) within the catalytic site of TYR. Finally, the cellular internalization and toxicity profile of the new synthesized molecules have been evaluated in NIH/3T3 fibroblast cell line.

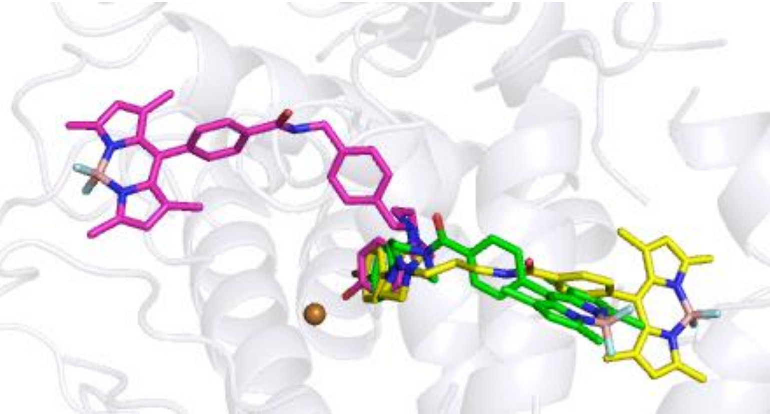

Figure 1. Superimposition of the synthetized compounds in AbTYR catalytic pocket.

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PO34

New mutual prodrugs of 5-fluorouracil and heme oxygenase 1 inhibitor with antiproliferative effects on breast cancer cells

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The 5-fluorouracil (5-FU) is an antimetabolite agent included in the WHO list of essential medicines; however, its anticancer efficacy is counteracted by high nonspecific toxicity and poor drug-likeness.[1] To overcome these drawbacks the development of mutual prodrugs of 5-FU is emerging as a promising strategy.[2] Heme oxygenase 1 (HO-1) is a stress-inducible enzyme responsible for the catabolism of heme. High levels of HO-1, in certain types of tumors, have been linked to cancer progression, tumor growth, and resistance to chemotherapy. Therefore, inhibition of HO-1, as a stand-alone or add-on cancer chemotherapy is emerging as an innovative pharmacological approach.[3]

Here we present the development of three new 5-FU/HO-1inhibitor mutual prodrugs bearing the 5-FU moiety linked to an arylethanoltriazole derivative (**LS 8/66**), recently identified for its greater inhibitory potency against HO-1 (HO-1 IC_{50} = 0.531 μM). Specifically, derivatives **SI 3/02** and **SI 3/08** (Figure 1) are characterized by the presence of succinic and glutaric linkers, respectively. Differently, compound **SI 3/07** (Figure 1) is a monoester derivative in which 5-fluorouracil-1-yl acetic acid was introduced instead of hydroxymethyl-5-FU to improve the metabolic stability. Finally, newly synthesized compounds were preliminarily tested to evaluate their *in vitro* effects on cell viability towards selected breast carcinoma cell lines.

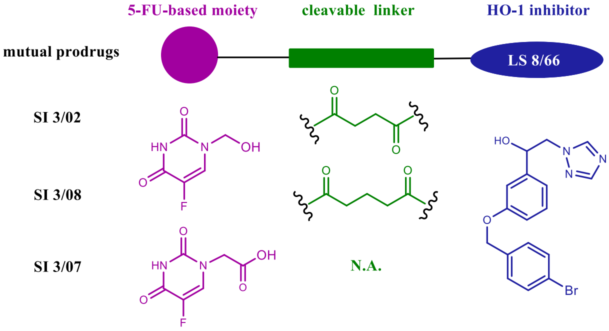

Figure 1. The general structure of newly synthesized 5-FU/HO-1 inhibitor mutual prodrugs.

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PO35

Synthesis of novel graphene-based materials for CO_2 capture

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With the current high consumption of fossil fuels and the rapid increase in atmospheric CO_2 concentrations, there is a strong need for energy efficient and selective capture of CO_2 from fossil-fuelled power plants and other large industrial sources[1]. Graphene based materials (G) are recently proposed like CO_2 adsorbent compounds due to their planar geometry, large surface area, versatile surface chemistry and tuneable structure[2]. In this way the preparation of G porous structures with pores' radii large enough to admit CO_2, allowed to obtain graphene derivatives with concomitantly high CO_2 selectivity and high absorption capacity [3]. All of this makes graphene materials an attractive alternative compared to the conventional CO_2 separation technologies.

Herein, we developed two nanoporous graphene oxide (nGO) systems one starting from graphite industries waste and the second one from commercial GO. Both nGO were suitably derivatized with tetraethylene pentaamine (TEPA) to incorporate amino groups, well known for their affinity towards CO_2. Their structure, morphology and chemical composition were investigated by several diagnostic techniques such as micro-Raman and X-ray photoelectron spectroscopies, thermogravimetric analysis (TGA) and scanning electron microscopy (SEM). To investigate the capacity of these novel graphene compounds to adsorb and release CO_2 under mild conditions, a pivotal aspect for ecological sustainability and energy efficiency, preliminary adsorption experiments at different temperatures and pressures were performed.

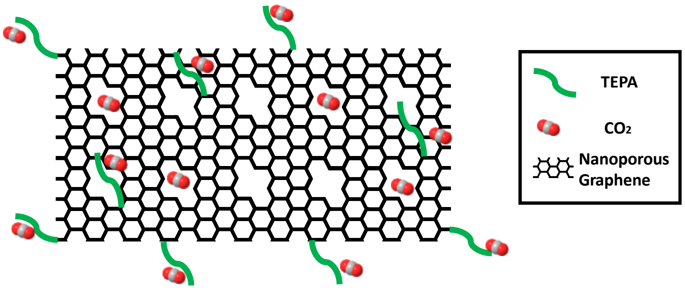

Figure 1. Representation of CO_2 molecules absorbed on the porous (TEPA) grafted graphene.

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PO36

Identification of new small molecules as correctors of CFTR with F508del mutation in the treatment of cystic fibrosis

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D. Guidone,[2] M. Genovese,[2] M.V. Raimondi,[1] V. Spanò, [1]A. Montalbano,[1,*] F. Ortuso,[3] S. Alcaro,[3]
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Cystic fibrosis (CF) is a genetic disease caused by mutations that impair the function of the CFTR chloride channel. This defect can be overcome by CFTR "correctors" that stabilize misfolded protein and increase membrane expression.[1-3] Although significant advances have been obtained by combinations of correctors with complementary mechanism, new modulators are still needed to maximize the rescue of F508del and other CFTR mutants with trafficking defects. Supported by Italian Cystic Fibrosis Foundation, we have identified a new class of small molecules (PP compounds), as CFTR correctors with high efficacy in the rescue of F508del-CFTR on native epithelial cells of CF patients particularly in combination with class 1 correctors (VX-809). By iterative cycles of chemical synthesis we focused on a multiparametric optimization of potency/efficacy and drug-like properties, in order to obtain candidates for preclinical and clinical development.[4] The new compounds were tested on cells with stable expression of mutant CFTR and the halide-sensitive yellow fluorescent protein (HS-YFP). The most active compounds were then validated in short-circuit recordings on primary airway epithelial cells (bronchial and/or nasal) and in biochemical and microscopy assays to evaluate CFTR maturation/trafficking. In combination with VX-809, the best compounds amplify the rescue by four/five-fold. Compounds PP028 and PP209, in agreement with dose-response relationships obtained with the HS-YFP assay on CFBE41o- cells emerged as particularly potent, being highly effective at 1 μM. Insight in the mechanism of action indicated that PP compounds act as class 3 correctors, since they induce synergistic effect when combined with class 1 (VX-809) and 2 (3151) correctors but not with class 3 (VX-445, 4172). In conclusion, the new class of compounds appear promising for the future development of combinatorial treatments for CF. This research is supported by the Italian Cystic Fibrosis Research Foundation (FFC#4/2018, FFC#3/2020 and Molecules 3.0). We acknowledge MUR (PNRR-M4C2-I1.3 Project PE_00000019 "HEAL ITALIA").

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PO37

Silver Fractal Platform: Synthesis and SERS Application for the detection of Biomolecules in Hydration Condition

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A highly sensitive method for detecting of biomolecules via Surface-Enhanced Raman Spectroscopy (SERS) has been exploited by using a plasmonic silver (Ag) dendrite platform. This 3D material is produced via metal-assisted chemical etching, resulting in a hierarchical structure composed of micro- and nano-cavities of varying sizes., This structure efficiently traps light across the whole visible spectrum, leading to the formation of numerous "hot spots" regions that significantly enhance the electromagnetic field. Additionally, the sponge-like behavior of the layer allows for the encapsulation and confinement of very small liquid sample volumes, enabling proteins to maintain their natural hydration shell and move freely within the fractal cavities. This facilitates the analysis of biomolecules in their biologically active conformation[1]. The SERS platform has been specifically applied to the identification of the Omicron variant of the SARS-CoV-2 virus, providing a detailed spectral fingerprint of nucleobases[2]. Furthermore, studies were also carried out to characterize, for the first time, the Raman spectra of three allergenic proteins from *Parietaria judaica*, leveraging the SERS "blinking" effect to gain insights into the proteins' vibrational modes[3].

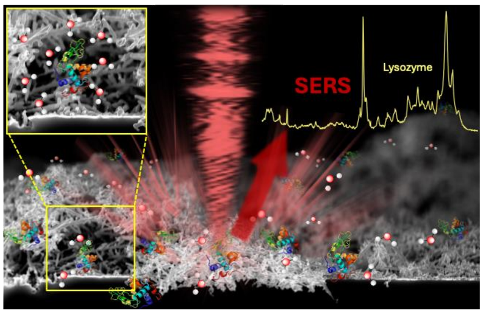

Figure 1. SERS Platform based on Ag dendrites confines the biomolecules (such as lysozyme, used as proof of principle) in liquid environment in micro/nano-cavities. When the laser beam is focused onto the platform it enhances the Raman spectrum.

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PO38

Mn-doped ZnO Nanoparticles: Synthesis, Characterization and Ti coating for Bone Tissue Regenerations

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The development of novel materials for bone tissue regeneration poses a significant challenge in biomedicine. Among the various materials, titanium (Ti) is the most common substance for bone implants, but they are vulnerable to infection. For this reason, functionalizing Ti surfaces could be a promising approach to improve both its antibacterial and biocompatibility properties. In this work we present a simple and rapid functionalization of Ti scaffolds by using colloidal ZnO and Mn-doped ZnO nanoparticles (NPs) to obtain materials with a continuous nanostructured film. [1] The ZnO and Mn-doped ZnO NPs, were characterized by using various techniques, including UV–vis spectroscopy, Transmission Electron Microscopy, Electron Energy Loss Spectroscopy, confirming Mn ion doping in the ZnO lattice. We evaluated its antibacterial activity against *P. aeruginosa* and *S. aureus*, and its biocompatibility using human fetal osteoblast cells, founding that Mn doping outperformed the undoped material. The results indicate that the new biomaterial exhibite strong antibacterial properties while maintaining high biocompatibility, [2] representing a significant advancement in the development of biomaterials for regenerative medicine applications.

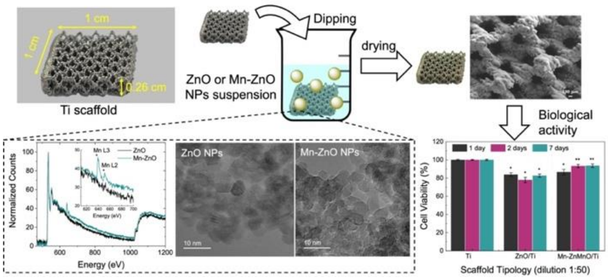

Figure 1. Coating of Ti scaffold with ZnO and Mn-doped ZnO NPs for osteo regeneration purposes. The use of spectroscopic and microscopic techniques has led to a complete characterization of the NPs.

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PO39

Methylated DNA Detection Based on Protein-Conjugated Magnetic Nanoparticles

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Magnetic nanoparticles (MNPs) emerged as innovative material in biomedical research due to their properties such as magnetization, biocompatibility, and chemical reactivity of their surface. Magnetic biosensing is one application that exploits the magnetization dynamics of MNPs to detect biomarkers in liquid samples[1]. Here, we investigate the capability of CoFeD nanoparticles functionalized with methyl binding domain (MBD) protein to detect methylated DNA. The magnetic characterization of both unmodified and MBD-functionalized CoFeD NPs, using AC magnetometer[2], showed a decrease of magnetization in the functionalized CoFeD NPs. However, the CoFeD-MBD NPs maintained sufficient magnetic properties for effective detection. Functional assays demonstrated the ability of CoFeD-MBD NPs to capture methylated DNA with a sensitivity of 100 pM, suggesting that MNPs could serve as a promising platform for biomolecule detection in cancer diagnostics.

Acknowledgments

This work received funding from the European Union's HORIZON-MSCA-2021-DN-01. STRIKE-101072462.

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PO40

Raman Spectroscopy and Neural Network for the Analysis of Berlin Wall Colors

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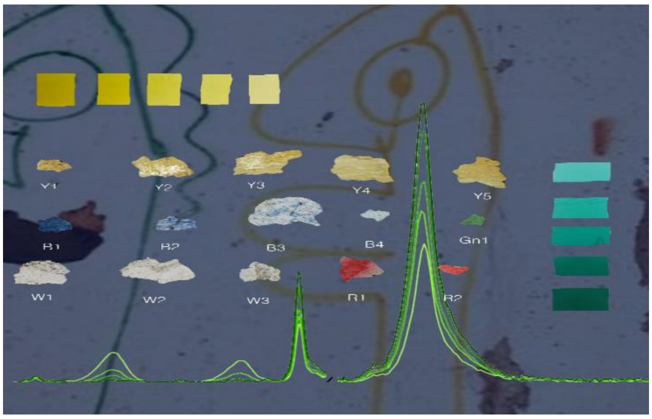
This research begins with the analysis of fragments from Berlin Wall street art to characterize the painting materials used. Spectroscopic results offer an overview of the painting techniques, but more importantly, they highlight a new advantage of applying Raman spectroscopy to the analysis of acrylic colors. The study demonstrates a correlation between peak intensity and compound concentration, leveraging the power of deep learning to quantify pigment mixtures in commercial acrylic products using Raman spectra collected with a handheld device (BRAVO by Bruker).

By employing a Convolutional Neural Network (CNN) algorithm[1], this study showcases the ability to analyze spectra and accurately predict the ratios of coloring compounds. Calibration and training reference materials were prepared by diluting commercial acrylic paints (Schmincke brand), mimicking the methods commonly used by street artists. For the first time, Raman spectroscopy offers valuable insights into calibrations for detecting dye dilution in commercial pigment mixtures, opening new possibilities for analytical quantification using handheld Raman spectrometers. This contributes to a deeper understanding of the materials and techniques employed by street artists.



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PO41

Analytical methodology for quantifying heavy metals in tattoo inks

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Several of the commercial tattoo inks contain heavy metal. Considered the limited literature data available on the concentrations of hazardous metals in products sold online or by street vendors, in this research, an analytical method was optimized to simultaneously quantify 18 elements in a complex matrix, such as tattoo inks, by inductively coupled plasma mass spectrometry (ICP-MS). Considering the quality parameters (linearity range, limits of detection and quantification, accuracy, precision, etc.), the method is suitable for the quantitative determination of the considered elements in tattoo ink samples.

The results showed that the contribution of metals to the compositions of tattoo inks was highly variable between samples, brands and even between inks of similar colour. Zinc, barium and manganese were the main metals. The total metal concentrations in the 16 tattoo ink analysed samples ranged from 0.060 to 16.9 mg kg^{-1}. Zinc is the element present in all samples, in fact, its concentration ranges from 3.4 to 13882 mg kg^{-1}. In three of the 16 analysed samples, zinc exceed those established by legislation (2000 µg g^{-1}). The concentration of Cr in all cases is higher than that permitted (0.5 µg g^{-1}). Considering the limit values, four of the analysed samples should not be used by tattoo artists. Our data indicate that the use in the tattooing process of several inks acquired on line at low cost might pose serious risks for the development of dermatological pathologies in tattooed people.

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PO42

Crystal structure of *C*-undecyl-resorcin[4]arene and dimethyl sulfoxide: solvate or cocrystal?§

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The hexameric resorcinarene capsule, first reported in 1997[1], has been the subject of a number of studies concerning supramolecular catalysis in confinement.[2] While the capsule self-assembly and catalytic activity is nowadays routinely investigated through NMR spectroscopy, XRD structural data of this kind of systems are limited to one pioneering example.[1] In the framework of the PRIN 2022 project "*Supramolecular catalysis in self-organized containers* – CAGED", we have been recently investing our energies into the crystallization of the large hexameric capsule based on the *C*-undecyl-resorcin[4]arene. In the course of our crystallization studies, we came across a new, peculiar, layered structure of *C*-undecyl-resorcin[4]arene. The novelty of such structure does not reside on the packing motif, which is indeed "old", meaning very similar to that observed in the presence of other solvent molecules,[3,4] but rather in the fact that DMSO is notoriously a non-solvent for the *C*-undecyl-resorcin[4]arene. For this reason, the new structure could be defined as a cocrystal of *C*-undecyl-resorcin[4]arene and DMSO, rather than as yet another *C*-undecyl-resorcin[4]arene solvate. This apparently small result of purely crystallographic interest is already opening new horizons in the investigation of the molecular recognition properties of large host molecules.

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PO43

The impact of counter-anions on aggregation kinetics and supramolecular chirality of a novel cyanine dye

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Non-covalent approaches are proving to be an efficient strategy for constructing supramolecular arrays with specific electronic and chiral properties. Among these architectures, J-aggregates of organic dyes stand out due to their red-shifted absorption bands relative to the monomer and their ability to widely distribute excitons. This makes them highly promising for diverse applications in organic materials developed through supramolecular methodologies.[1]

In this work, we present the synthesis, full characterization, and comprehensive study of the aggregation kinetics of a novel J-aggregating chiral derivative of TDBC dye (*Figure 1a*). We demonstrated that kinetic parameters significantly influence the expression of chirality in J-aggregates, revealing a correlation between the kinetics of the aggregation process and the optical properties of the final assemblies.[2] Additionally, we observed that varying the type of salt used to promote dye aggregation leads to the formation of species with distinct absorption features (*Figure 1b*). These morphological variations are closely related to the structure-making or structure-breaking abilities of different anions and their influence on the solvent's hydrogen bonding network.[3] The correlation between the position of the J-aggregates band and the sign of the circular dichroism (CD) bands with the hydrogen bonding capabilities of the anions suggests changes in electronic coupling and potentially in the morphology of the aggregates in solution, paving the way for new insights into further structural characterization of these species.

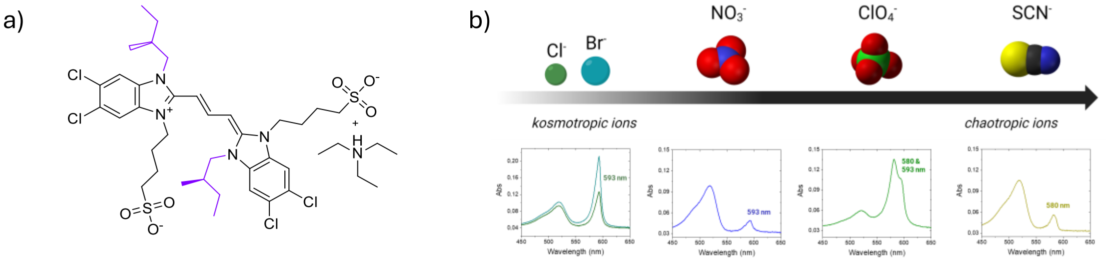

Figure 3 a) Chemical structure of the TDBC derivative b) The effect of the counter-anions on the position of the J-aggregates absorption band

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PO44

Pharmacophore-based virtual screening for the identification of a new elastase inhibitor for anti-ageing purposes

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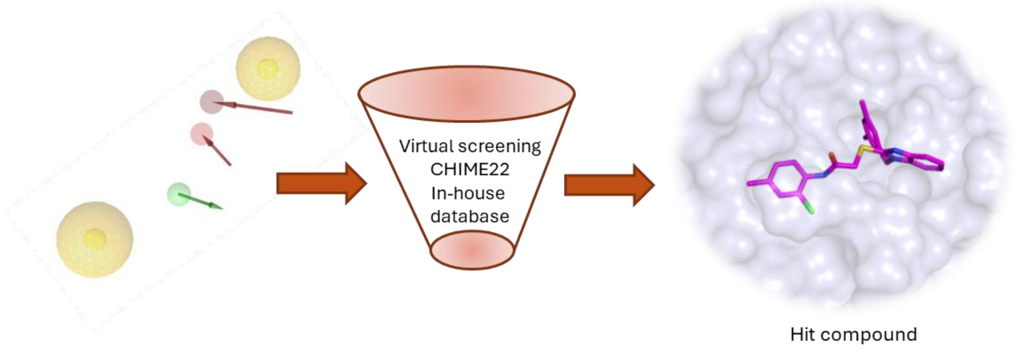
Skin ageing is a natural process influenced by intrinsic factors such as age, genetics, hormonal changes, metabolism, and extrinsic factors that include UV radiation, environmental pollution, smoking, poor diet.[1] The process of skin ageing is also represented by the formation of wrinkles due to the loss of elasticity and resilience of the connective tissue. This phenomenon is due to the action of the elastase enzyme, which degrades elastin fibres.[2] Elastase inhibitors can increase skin elasticity, preventing the formation of wrinkles and sagging skin. In this study, a computational approach made it possible to identify a non-peptide inhibitor of elastase. Initially, through a structure-based approach, pharmacophore hypotheses were developed, which were subjected to refinement using alanine scanning and molecular dynamics simulations. A simplified model was then obtained, which was used to perform virtual screening of an in-house library (CHIME22). One compound was found to be a new interesting elastase inhibitor that could be used as a hit in the search for novel, more efficient ligands. In order to evaluate the binding mode at the active site, molecular docking studies on elastase enzyme were also performed on our hit compound.



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PO45

Sicilian cultivars' grape seed proteins: extraction, characterization and wine fining application.

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In this research, chemical composition of grape seeds belonging to four different cultivars endemic to Sicily has been investigate and protein extracts was tested to evaluate their use as clarifying agents. The wine-making industry constitutes one of the most important agro-industrial sectors worldwide. However, the wine industry produces, as other industrial processing of plant-based food[1] in a short period of time, a large amount of waste and by-products, including grape seeds, representing about 30% of the initial weight of the grapes. Food waste production is a global problem due to its impact on the environment and the economy, so reducing it is crucial to achieving sustainable development[2]. In this context, grape seeds from Catarratto, Inzolia, Pinot Nero, and Petit Verdot cultivar have been extracted by a multistep process and the extracts have been characterized. Electrophoretic analysis of protein extracts revealed the presence of albumins as the main class, followed by globulins and prolamin (Figure 1). In order to assess the possible clarifying effect of the protein extracts obtained, tests were carried out on wine samples by evaluating the decrease in turbidity. All samples showed a good effect in reducing wine turbidity, highlighting the possible application of these extracts as endogenous clarifying agents.

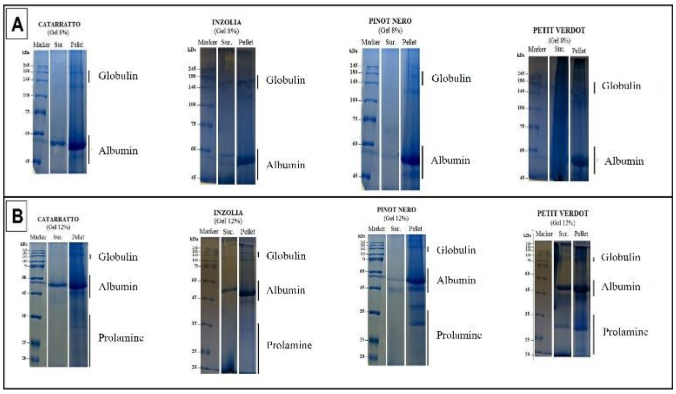

Figure 1. Electrophoretic analysis with Coomassie Blue staining A) Gel prepared with 8% polyacrylamide B) Gelprepared with 12% polyacrylamide.

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PO46

Recovery of *Critical Raw Materials*: a comparison between various waste biomasses

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This study presents the preliminary results obtained by using waste biomasses from the industrial food chain to develop multifunctional materials capable of efficiently and selectively detecting, binding, and extracting rare earth metal cations from aqueous solutions simulating real matrices. These metals are classified as "*Critical Raw Materials*," a group of elements whose recovery is considered strategic by the European Community [1]. The use of agri-food industry wastes as secondary raw materials offers a sustainable and environmentally friendly approach that could be beneficial for the possible recovery of rare earth metals. Specifically, the adsorption of neodymium (III) and dysprosium (III) ions from aqueous solution was investigated at the pH range 3.0-5.0 and t = 25°C, using different waste biomasses, namely Bergamot Pomace (BP), Olive Pomace (OP), and Grape Pomace (GP), chemically pretreated at t = 30°C with H_2O and 0.10 mol dm^{-3} HNO_3 [2,3]. The materials were characterized using various analytical techniques. FT-IR ATR spectroscopy [2] confirmed the presence of functional groups capable of interacting with the aforementioned metals. Batch experiments were conducted to assess their adsorption capacity in solutions containing the metal ions (M^{3+} = Nd^{3+}, Dy^{3+}), with the M^{3+} concentrations determined by ICP-OES [[4]]. The results from the adsorption experiments showed that the Langmuir equation provided the best fitting isotherm model for BP, OP, and GP in rare earth metal adsorption. The recovery of metals adsorbed on the biomasses was carried out using HNO_3, although the reused materials exhibited lower performances if compared to the initial ones, except for BP, which demonstrated excellent reutilization capacity [4].

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PO47

Highly efficient bio-inorganic fabric coatings towards improved sustainability of the textile supply chain

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Functional coatings for fabrics play a critical role in modern society by enhancing the performance and durability of textiles. These coatings provide protective properties such as water resistance, UV protection, stain repellency, and antimicrobial features, which are essential in industries like healthcare, wellness, as well as indoor/outdoor apparel. They may also contribute to sustainability of the textile supply chain by extending the lifespan of fabrics, reducing the need for frequent washing, and minimizing environmental impact. In addition, functional coatings enable the development of smart and high-technological textiles for a wide series of applications, including wearable electronics, still improving overall performance and quality of product-life through innovation in comfort, safety, and convenience[1]. To make functional coatings for fabrics more sustainable, the shift to bio-inorganic raw materials is crucial. Using renewable resources like plant oils, starch, and cellulose can replace petroleum-derived chemicals, reducing environmental impact. These materials are water-based, biodegradable and offer a lower carbon footprint. Additionally, innovations in green chemistry can optimize production processes, minimizing waste and energy consumption. By enhancing the durability of bio-based coatings, fabrics can maintain their protective properties over time, reducing the need for frequent replacement[2]. Collaboration between industries and research institutions can drive the development of bio-based polymers and nanomaterials, fostering sustainable textile production on a larger scale.

This work outlines the creation of novel hybrid nanostructured materials through various chemical synthesis approaches, including combining bio-based polymers like alginate, chitosan, and cellulose with synthetic or blended polymers and functional nanomaterials (i.e. clays) or molecules. Eco-friendly and green synthesis methods, utilizing bio-based, natural, or waste-derived reactants, were also employed to produce more sustainable multifunctional hybrids or nanostructured textile coatings with tailor-made properties aligned with circular economy principles. Additionally, the chemical, physical, and morphological characteristics of all the precursors, materials, functional coatings, and treated textiles are discussed.

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PO48

Production of hydrophilic polyvinylidene fluoride/alkali lignin membranes and their biofunctionalization

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Polyvinylidene fluoride (PVDF) is one of the most widely used polymers in membrane manufacturing due to its excellent properties (including chemical, thermal and mechanical resistance). However, when PVDF membrane is used to separate nonpolar compounds from aqueous streams, the hydrophobic nature causes sticking and spreading of hydrophobic material on the membrane surface, causing significant pore clogging and abatement of membrane performance. The main approaches used to hydrophilize PVDF membranes are grafting, coating and blending. In this work, the strategy was to hydrophilize PVDF during the preparation process by mixing it with alkali lignin (AL) in the pot[1]. This method aimed to streamline the production by reducing the number of steps compared with post-processing methods such as grafting or coating. The presence of hydrophobic/hydrophilic groups in the AL structure addressed the challenge of compatibility between PVDF and conventional hydrophilic polymers, improving the interaction between the components. Highly hydrophilic membranes consisting of an adjusted PVDF/AL polymer ratio with robust mechanical stability were produced. Characterization methods confirmed the suitability of the new blended mixture for membrane preparation and its hydrophilic nature. The obtained material showed an improved pure water permeance and demonstrated resistance to irreversible fouling. The membrane's ability to treat wastewater streams and its resistance to fouling were confirmed by separating stable and uniform submicron-sized oil-water emulsions with high rejection (>99.9%) up to a volume reduction factor of 7.7.

For this remarkable performance, the new hydrophilic membranes have been used as a biofunctionalization support for the anchoring of phosphotriesterase (PTE) enzyme *via* a covalent bond[2]. PTE was chosen as a model biomolecule to study the binding capacity and catalytic properties of engineered membranes for the use in decontamination of water from toxic substances such as organophosphate pesticides (e.g., paraoxon).

The lecture will illustrate the performance of PVDF/AL membranes in the treatment of wastewater solutions and their use as support materials for the attachment of biomolecules.

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PO49

Coupling of an electrosurgical knife with direct mass spectrometry for the rapid discrimination of tumors based on lipidomic profile

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Rapid Evaporative Ionization Mass Spectrometry (REIMS) is an emerging ambient ionization technique which allows the identification of tissues in real-time through the analysis of the informative aerosols generated during their intraoperative electrosurgical dissection. The coupling of REIMS with a surgical electrocautery is known as the intelligent knife (iKnife)[1]. The MS spectra obtained are used to build predictive statistical models, which allows the immediate identification and differentiation of tissues based on their differences in the lipidomic profiles[1]. Currently, REIMS technology has been validated for metabolic phenotyping tumors intraoperatively in human surgical oncology, exhibiting high diagnostic accuracy, improving margin assessment and surgical outcomes[2,3].On this basis, the aim of this talk is to underline the power of the iknife tool in both veterinary and human medicine areas. More in details, the application in neurosurgery will be presented to demonstrate the potentiality of REIMS in the identification of brain tumor grade and type, which can be exploited for an early cancer diagnosis. An accuracy higher than 91% was achieved with a low percentage of both false positives and false negatives. Glycolipids, phospholipids (PLs) and sphingolipids were identified as discriminant features. The increase of PLs in tumor tissues is the consequence of an enhanced synthetic activity during carcinogenesis, whereas the upregulation of glycoceramides in drug-resistant tumor is the way by which tumor cells can improve their survival. In the veterinary field, different statistical models were built to reliably identify several mammary gland pathologies, including benign and malignant canine mammary tumours (CMTs), which were also remarkably differentiated based on changes in cellular metabolic phenotype during neoplastic transformation. The results demonstrated that REIMS is effective in identifying neoplastic tissues with an accuracy of 97%, with differences in MS spectra characterized by the relative abundance of PLs compared to triglycerides more commonly identified in normal mammary glands.

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PO50

Non-covalent interactions of a cationic porphyrin with anionic carboxymethyl cellulose

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Carboxymethyl cellulose (CMC), a cellulose derivative, has emerged as one of the most promising polymers due to its versatile set of properties.[1] CMC, in fact, acts as a powerful chelator, binding metal ions to itself and removing them from solution. Its chemical structure, characterized by the presence of carboxymethyl groups, gives it excellent adsorption capacity, making it particularly effective in removing heavy metal pollutants such as copper, nickel, and zinc from water[2].

In this work, we investigated the interaction between CMC and 5,15-bis(4-n-methylpyridyl)-10,20-diphenylporphyrin (t-H_2Pagg) and its metal derivatives to develop potential new sensors for heavy metals. Experiments using spectroscopic techniques such as UV/Vis, fluorescence, resonant light scattering and circular dichroism, show that the affinity between CMC and metal porphyrins is strongly influenced by the nature of the metal and its coordination geometry.[3] These selective interactions open promising prospects for the design of fluorometric sensors capable of detecting specific metals in complex matrices, such as contaminated waters.

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PO51

Functional high-performing clay-based sensing fabrics as efficient tools for sustainable applications

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In recent years, the ever-increasing interest in real-time monitoring of environmental pollutants and parameters has pushed the scientific world to encourage research on the development of optical portable colorimetric sensors for parameters and contaminants detection.

In particular, colorimetric sensors show promising potential for the sensing of metal ions, organic dyes, drugs, pesticides and other toxic pollutants, due to their easy fabrication, rapid and naked-eye detection, and high sensitivity.

In this context, molecules which change chemically and reversibly in response to one or more external stimuli are of particular interest, as well as technologies that allow their integration into polymers for smart textiles or werable sensors use[1]. Among the latter, the sol-gel technique is among the most sustainable, promising and versatile and allows to immobilize organic functional molecules covalently or through weak interactions through hydrolysis and condensation reactions of metal precursors[2].

In this work, through the sol-gel technique a hybrid textile for pH-sensing applications was designed; in particular, a user-friendly innovative and sustainable sensing system that may either respond colorimetrically to the presence of various environmentally parameters (such as pH), was developed using different chromophores.

The functional hybrid material synthesis is described, as based on functionalized clay successful used to immobilize different organic dyes and as applied on cotton fabrics.

Finally, their employment for the pH variation detection is shown, together with preliminary tests for validation in relevant laboratory environment.

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PO52

Valorization of calabrian ancient grains

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Wheat, a member of the genus *Triticum* of the *Poaceae* family, has long been consistently used for the production of flour, pasta and bread. The ever-increasing demand of consumers and the large-scale and environmentally unsustainable cultivation of this agricultural product have resulted in wheats of poor nutritional quality[1]. The latter has contributed to increase the onset of chronic degenerative diseases and intolerances or aggravate pre-existing disease conditions[2]. Consequently, an urgent need to cultivate healthier grains with excellent nutritional qualities, using environmentally sustainable techniques, has been recorded. In this context, the scientific attention has been focused on ancient grains, cultivated using traditional processing techniques, rich in carotenoids, vitamin E, phytosterols and other bioactive compounds[3]. Herein, the nutritional and nutraceutical properties of four different ancient grains cultivars (Senatore Cappelli, Verna, Maiorca, Gentilrosso), grown in Calabria by the "Società Agricola Mulinum s.r.l." (San Floro, Catanzaro, Italy), were studied and compared with three commercial wheat varieties. The wheat extracts were obtained by ultrasonic-assisted extraction, using three different environmentally friendly solvents: ethyl acetate (EA), ethanol (E) and water (W). The antioxidant and anti-inflammatory activities of all the samples were evaluated through *in vitro* experimental procedures. The obtained results highlight the health and nutritional benefits of ancient grains and encourage further research.

Figure 1. Ancient grains, Società Agricola Mulinum s.r.l. (San Floro, Catanzaro, Italy).

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PO53

Innovative Nanostructured Materials for Portable Sensors in On-Site Heavy Metal Detection

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Pollution from heavy metal ions, such as lead, mercury and cadmium, poses a growing threat to the environment and human health. These metals can accumulate in ecosystems and the food chain, contaminating soil, water and food products. The consequences for human health include neurological problems, respiratory diseases and reproductive disorders, making it urgent to monitor and detect these substances effectively. In recent years, research has focused on developing more sophisticated and accessible detection methods.[1] Traditional analytical methods, such as mass spectrometry and chromatography, are expensive and complex. In response, portable, lightweight and easy-to-use sensors have been developed that enable on-site measurements and reduce waiting times. Optical sensors enable rapid detection of pollutants in freshwater and wastewater, which is useful in precision agriculture, even for those without specific expertise. In addition, the use of advanced nanomaterials improves sensitivity and selectivity, ensuring accurate measurements under various conditions. In this context, we will explore the innovation of smart and functional nanostructured materials created for optoelectronic applications in heavy metal monitoring. For example, an optoelectronic sensor designed for irrigation water is capable of detecting and quantifying the presence of harmful heavy metals in the water used for crops. These devices, which integrate optical and electronic technology, provide detailed water quality analysis. The information collected can be sent and processed in real time, allowing farmers and other users to constantly monitor the quality of irrigation water and take rapid action if safety limits are exceeded. Thanks to these advanced technologies, farmers can protect their crops from potential contamination, ensuring the production of safe and healthy food.[2] Furthermore, secondary or bio-based materials derived from agricultural waste are frequently used, aligning with the principles of the circular economy and zero-waste practices, which promotes greater sustainability and a more environmentally friendly approach to high precision agriculture.

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PO54

New photovoltaic device based on natural microbial pigments co-sensitization

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Developing innovative dye sensitized solar cells based on microbial pigments, is very important to meet the demands of sustainable photovoltaic devices. With this purpose, microbial extracts obtained from *Talaromyces atroroseus* GH2, *Arthrobacter bussei* CP30 and *Paracoccus bogoriensis* BOG6 cultivations, have been used in this study. The extracted pigments were tested to evaluate their suitability as photosensitizers through co-sensitization method. UV–vis measurements were carried out to determine the absorbance intensity, while Photoelectrochemical and Electrochemical Impedance Spectroscopy (EIS) analyses were applied to evaluate the devices' photovoltaic parameters and impedance characteristics. The best device, obtained by the co-sensitization of the dyes produced by *Talaromyces atroroseus* GH2/*Paracoccus bogoriensis* BOG6, exhibited a Jsc of 1.59 mA/cm^2, Voc of 0.35 V, FF of 0.62, and a PCE of 0.34 %. This study highlights the potential of microbial-derived pigments in the development of DSSCs.

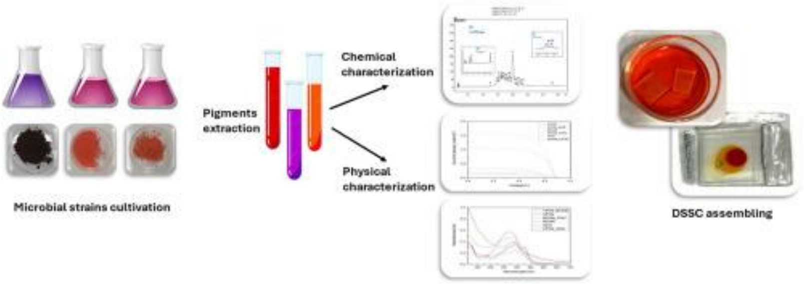

Figure 1. *Photovoltaic device development scheme*

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PO55

Design, synthesis and biological evaluation of novel antiviral agents for the treatment of Dengue and Zika virus infections

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Neglected Tropical Diseases (NTDs) includes 20 different infections that are prevalent in tropical areas, where they affect poor communities, women and children. Two NTDs are those caused by the Dengue (DENV) and Zika (ZIKV) viruses. DENV can lead to fatal haemorrhagic fever while ZIKV causes Guillain-Barré syndrome in adults. Unfortunately, approved vaccines (DENGVAXIA and QDENGA) present several limitations. In the present scenario, NS2B/NS3, the main serine protease of DENV and ZIKV is considered a promising target for the development of specific anti-flavivirus therapies [1]. Our research is focused into the development of novel antiviral agents targeting NS2B/NS3 serine protease; currently, our work involves the batch synthesis of allosteric inhibitors starting from the lead compound **1** (Figure 1) [2] which inhibits the serine protease of DENV and ZIKV with IC_{50} values of 8.58 µM and 0.93 µM, respectively. An extensive study of the structure-activity relationship (SAR) has been carried out concerning the variation of the three critical portions of the molecule, i.e. the benzothiazole nucleus, that bears two hydroxyl groups, the proline residue and the aromatic region anchored to the sulfonyl group. The role of the benzothiazole ring has been evaluated through its replacement with other heterocyclic nuclei such as the benzimidazole. We investigated the role of the proline residue stereochemistry on the inhibitory properties by synthesizing both the *R* and *S* enantiomers for the most promising inhibitors. In addition, the sulphonyl has been replaced with a carbonyl group to investigate its ability to establish interactions with the allosteric site, while the nitro group present at position 4 of the aromatic ring has been replaced with different electron-withdrawing substituents in *ortho*, *meta* or *para* position, to evaluate the impact on antiviral activity. All the synthesized inhibitors have been tested against NS2B/NS3 of DENV and ZIKV and the results will be presented and discussed.

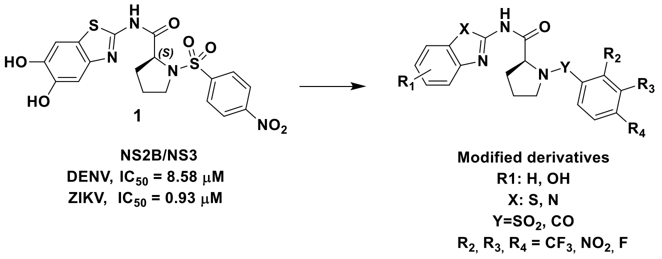

Figure 1. Design of novel inhibitors of NS2B/NS3 serine protease of DENV and ZIKV.

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PO56

Novel Pt(II) and Ru(II) complexes: synthesis and interaction with G-Quadruplex structures

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G-quadruplexes (G4s) are DNA secondary structures involved in key biological functions like transcription, translation, genome stability, and cancer.[1] Recent findings have shown that G4s also form in mitochondrial DNA (mtDNA), hinting at a potential role in mitochondrial regulation.[2] Schiff base metal complexes of the Salphen type, along with polypyridyl complexes containing the dipyrido[3,2-a:2',3'-c]phenazine (dppz) ligand, have been shown to interact efficiently with G4s.[3],[4] To explore the effects of G4-targeting compounds on mtDNA G4s, we synthesized a Pt(II) Salphen complex and Ru(II) complexes of the type [Ru(bipy)$_2$(L)] and [Ru(phen)$_2$(L)], where 'L' is a dppz unit modified with a triphenyl phosphonium salt. Additionally, given the promising yet underexplored anticancer properties of metal complexes with oxadiazole ligands, we investigated their G4 interaction in new Ru(II) complexes containing 1,2,4-oxadiazole ligands. Various spectroscopic techniques, including UV-Vis absorption, fluorescence, circular dichroism, and FRET, were used to evaluate their interaction with genomic and mitochondrial G4 sequences.

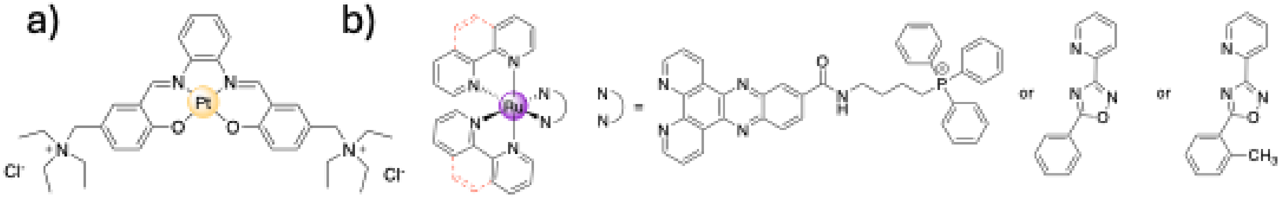

Figure 1. Structure of the synthesized platinum (a) and (b) ruthenium compounds

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PO57

Catalytic Upcycling of Polyolefin Waste into Value-Added Liquid Alkanes

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Each year, millions of tons of mismanaged plastic waste accumulate in the environment, creating major ecological challenges. This issue is particularly acute with polyolefins (POs), where 95% of post-consumer POs become waste, making up over 60% of the plastic content in municipal solid waste.

The low recycling rates of POs represent a significant missed opportunity in the plastic market, running counter to the goals outlined in the "European Strategy for Plastics in a Circular Economy." Although EU directives call for innovative approaches, such as upcycling plastic waste into valuable chemicals and fuels, the upcycling of POs waste remains at an early stage. This project seeks to enhance awareness and drive progress in the catalytic upcycling of POs waste into valuable liquid alkanes. The research will focus on identifying key catalyst properties and process parameters that influence the selective cleavage of C-C bonds in POs.Two types of catalysts—one with acid sites and the other with ruthenium nanoparticles—will be developed and rigorously evaluated against a commercial standard. Various polyolefin samples will be subjected to reductive conditions, including hydrocracking and hydrogenolysis, as well as transfer reductive conditions using aliphatic alcohols as mild hydrogen donors.

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PO58

Assessment of consolidation treatments for fresco and mud bricks using nanostructure systems

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Intervention strategies for the treatment of cultural assets located in environments where thermo-hygrometric conditions are critical for their conservation have always been a challenge for restorers. Hypogeal environments and archaeological sites are environments where environmental parameters are difficult to control and where the conservation status of artefacts is usually compromised. The present contribution aims to present the results obtained from the study carried out on two Sicilian case studies: the frescoes located at the Complex of S. Maria della Grotta (TP)[1] and the mud bricks of the Solunto (PA)[2] buildings. The study involved several phases; as every good conservation project envisages, it was essential to first draw up the state of conservation of the artefact contextualised in its archaeological context. A second phase involved the use of diagnostic techniques aimed at gaining knowledge of the constituent material, substrates and degradation phenomena encountered.

Figure 1. Application of nanomaterials on a mud brick.

The information gathered made it possible to correctly define and develop the nanostructured systems to be tested and the application methods [3,4]. Finally, the most promising nanostructured systems were tested in the laboratory on mock ups made ad hoc and aged simulating a real context and later, in situ, with the aim of stopping, or as much as possible slowing down, the phenomenon of degradation taking place on the artefact.

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PO59

Dry Reforming of Methane over Ni-based Catalyst: Influence of MgO Support and MgO Doping with Fe, Cu, and Ce

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Dry reforming of methane (DRM) is a promising catalytic process that converts two major greenhouse gases, methane (CH_4) and carbon dioxide (CO_2), into syngas (a mixture of CO and H_2). This offers a pathway for sustainable fuel production while addressing environmental concerns.[1] However, DRM faces challenges due to side reactions, such as methane decomposition, Boudouard reaction, reverse water–gas shift and CO reduction, all leading to carbon deposition and catalyst deactivation. Ni-based catalysts are widely used in DRM because of their cost-efficiency and strong CH_4 activation properties; however, their performance can degrade over time due to sintering and coke buildup at elevated temperatures. To enhance their stability and improve the catalytic activity the chemical composition of the supports and the preparation method are crucial.[2] This study focuses on evaluating the catalytic performance of Ni supported on magnesium oxide and MgO doped with iron, copper and cerium in the DRM reaction (Figure 1). The influence of dopants on the reduction properties, structural phase composition and on the catalytic activity was investigated. Characterizations of the catalysts by XRD and TGA-DSC were conducted after the DRM reaction to assess any modification of the structural properties and eventual coke formation and decomposition temperature. The results aim to provide insights into the optimization of support materials to improve the durability and efficiency of Ni-based catalysts in DRM, contributing to increase the sustainability of syngas production.

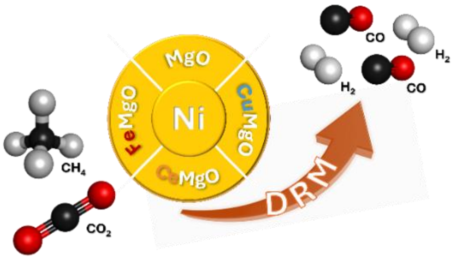

Figure 1. Schematic representation of the DRM reaction carried out over Nickel catalysts supported on MgO and MgO doped with Fe, Cu and Ce.

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PO60

Machine Learning techniques for GLUT-1 inhibitors discovery

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The identification of novel inhibitors targeting the membrane transporter GLUT-1 represents a promising approach in cancer therapy, as GLUT-1 plays a pivotal role in glucose uptake by tumor cells. Targeting GLUT-1 aiming at disrupting the increased metabolic demands of cancer cells, offers a strategic antitumor intervention. This study employs Machine Learning (ML) methodologies to develop a predictive model for the activity of novel, yet-to-be-synthesized, compounds. The results of this model analysis allow to identify molecular substructures that correlate with enhanced inhibitory activity, guiding the design and optimization of existing compounds. A Random Forest Classifier was employed to predict compound activity with high accuracy, using interpretable molecular descriptors related to specific functional groups. A Decision Tree was also utilized to extract key features contributing to inhibitor activity (**Figure 1**). These findings support the rational design of more effective GLUT-1 inhibitors, advancing therapeutic development.

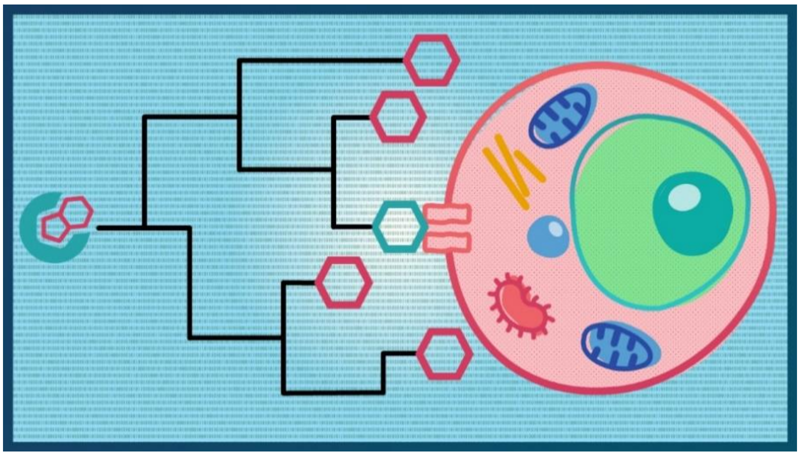

Figure 1. A Machine Learning model can be trained to identify effective inhibitors from extensive databases.

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PO61

Synthesis of 5-imino-3,5-dihydrofuro[3,4-*c*]isochromen-1-ones by Pd-Catalyzed Carbonylative Double Cyclization

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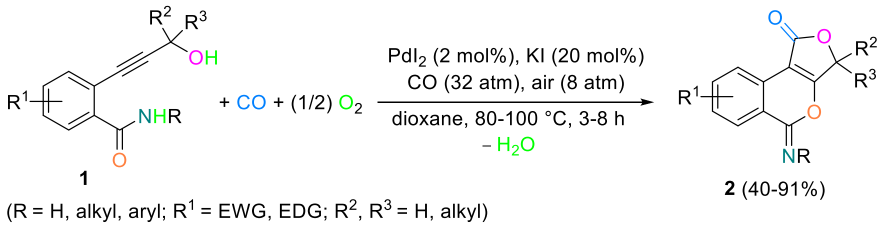
Carbonylation reactions are known to play a major role in the direct synthesis of carbonyl compounds of industrial interest as well as for the sustainable preparation of fine chemicals.[1] In particular, carbonylative double cyclizations are powerful synthetic methodologies that allow the construction of two new cycles in one synthetic procedure with formation of carbonylated polycyclic structures starting from suitably functionalized substrates.[2,3]

We report here a new carbonylative oxidative double cyclization process which leads to the formation of 5-imino-3,5-dihydrofuro[3,4-*c*]isochromen-1-ones **2** in one step starting from readily available 2-(3- hydroxyprop-1-yn-1-yl)benzamides **1**, CO and O_2 (from air) under the catalytic action of PdI_2 in conjuction with an excess of KI. Products are obtained in chemo- and regio-selective manner under relatively mild conditions (at 80-100 °C for 3-8 h under 40 atm of a 4:1 mixture CO-air) and with 40-91% isolated yields (*Scheme 1*)



Scheme 1

Tricyclic heterocycles **2** represent an interesting new class of polyheterocycles, with potential applications in different fields, including medicinal chemistry and material science. The structure of a representative product has been confirmed by X-ray crystallographic analysis.

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Giulia Maria Itri	**FC16,** OC16
Gabriele La Monica	**PO25,** PO7
Roberta La Tella	
Chiara La Torre	**FC15**
Roberto Laganà Vinci	
Gabriele Lando	FC11, PO9, PO21, PO24, PO46
Davide Lascari	**OC20,** PO46
Federica Leone	**PO26**
Giovanna Li Petri	**OC4**
Liliam Maria Liotta	**PO27**
Carmen Lo Sardo	**FC13**
Valeria Loise	**OC22**
Lisa Lombardo	**PO28**

Antonella Maggio	PO45
Angela Malara	
Raffaella Mancuso	**PO29,** OC28, FC23, PO61
Francesca Mancuso	
Giuseppe Marcì	**PO30,** OC16, PO18
Tiziana Marino	OC28, PO14
Maria Marra	**FC22**
Agostino Marrazzo	OC27, FC18, PO19
Annamaria Martorana	PO7, PO25
Paola Marzullo	**PO31**
Marina Massaro	FC1, PO26
Martina Mazzaferro	**PO32**
Antonino Mazzaglia	OC18
Gloria Mazzone	OC11
Federica Meringolo	**FC3**
Grazia Maria Lucia Messina	**PL2**
Demetrio Milea	
Marco Milone	**OC29,** PO32
Placido Mineo	FC1
Salvatore Mirabile	**PO33**
Sara Mocka	**PO34**
Fabricio Molinari	**PO35**
Luigi Mondello	OC17, PO10, PO49, PO54
Maura Monforte	**FC21**
Alessandra Montalbano	**PO36,** OC24
Vittorio Morandi	
Dario Morganti	**PO37, PO38**
Maria Grazia Musolino	**PL1,** OC1
Anna Maria Napoli	OC32, FC13
Beatriz Naranjo-Martinez	**PO39**
Giulia Neri	PO1, PO35
Angelo Nicosia	FC1
Giuseppe Nocito	**OC18**
Anna Notti	OC29, PO32
Mariangela Novello	**FC23**
Maria Antonietta Occhiuzzi	**OC9,** PO13
Santino Orecchio	PO41, FC12

Silvia Orecchio	**FC12,** PO41
Emilia Paone	FC16
Andrea Asia Paparella	**PO42,** OC22
Melchiorre Parisi	OC29, PO32
Barbara Parrino	**PL4**
Vincenzo Patamia	OC2, OC27
Teresa Pavaglianiti	**PO43**
Teresa Maria Pellicanò	
Ugo Perricone	
Dario Perziano	**OC3**
Alberto Pettignano	OC20, PO46
Anna Piperno	OC26, PO1, PO35, PO39
Giovanna Pitasi	**PO44,** PO33
Valeria Pittala	PO27, PO34
Maria Gaetana Giovanna Pittalà	**FC24,** FC20
Pierluigi Plastina	OC31
Maria Rosaria Plutino	FC10, PO47, PO51, PO53
Fortuna Ponte	**OC11**
Antonella Porrello	**PO45**
Mario Prejanò	OC28, PO14
Santo Previti	OC23, PO15
Giuseppe Proietto Salanitri	**OC19**
Salvatore Giovanni Michele Raccuia	**PO46,** PO21, PO24
Giovanna Raia	**OC30**
Giulia Rando	**PO47,** PO51, PO53
Serena Regina	**PO48**
Antonio Rescifina	OC2, OC14, OC27, FC18, PO19
Serena Riela	FC1, PO26
Francesca Rigano	**PO49**
Andrea Romeo	PO50
Chiara Rossini	
Beatrice Russo	**FC7**
Patrizio Russo	**OC28**
Erika Saccullo	**OC2**
Mariachiara Sarà	**PO50**
Ignazio Sardo	
Angela Scala	OC18, OC26

Elisabetta Scalone	**PO51**
Eva Scarcelli	**PO52**
Emanuele Luigi Sciuto	**FC9**
Stefano Scoditti	**FC8,** OC11
Silvia Sfameni	**PO53,** PO47, PO51
Emilia Sicilia	OC11, FC8
Maria Stefania Sinicropi	FC22, PO11, PO16, PO52
Donatella Spadaro	**PO54,** FC17, PO20
Josè Starvaggi	**PO55,** PO15
Alessio Terenzi	**PO56,** OC25
Elisabetta Grazia Tomarchio	**OC14**
Marco Francesco Torre	**OC15**
Antonio Cosimo Pio Trimboli	**PO57**
Chiara Tuccio	**PO58**
Laura Valentino	**PO59,** FC23
Filomena Vigliatore	
Vincenzo Vigna	**PO60**
Roberto Zagami	
Emanuele Zanda	**FC11,** PO21, PO46
Maria Zappalà	PO15, PO55
Ida Ziccarelli	**PO61,** FC23
Mariosimone Zoccali	**OC17**