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Sezione Toscana

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ECCELLENZA 2023-27

UNIVERSITA DEGLI STUDI FIRENZE
PhD
Chemical Sciences

Book of Abstracts

4th Edition of the Symposium

PhD in Chemical Sciences at UniFi

14th - 17th January 2025

Tue 14th: 14:00 – 17:15

Wed 15th: 9:00 – 16:30

Thu 16th: 9:00 – 16:30

Fri 17th: 9:30 – 16:00

Plesso Aule "Enrica Calabresi"

Room C3

Scientific Campus: Sesto Fiorentino

Via Edoardo Detti 3, 50019-Sesto F.no (FI)

4th Edition of the Symposium

PhD in Chemical Sciences at UniFi

PiCSU 2025

14th-17th January 2025, Sesto Fiorentino (FI), Italy

BOOK OF ABSTRACTS

Ideated and edited by:
Anna Maria Papini, Andrea Sodini, Lenardo Tacconi, Silvia Bracci, Matilde Rossi, Simone Ventisette, Samuele Baldini, Lapo Querci.

Organizing Commitee

Several students enrolled in the PhD program in Chemical Sciences volunteered to serve as members of the organizing committee for this symposium. The committee independently conceptualized and organized the event, making it accessible to all students of the University of Florence. This initiative provided PhD students in Chemical Sciences with an opportunity to share and discuss their research projects.

Andrea **Sodini**, XXXVIII cycle

Leonardo **Tacconi**, XXXVIII cycle

Silvia **Bracci**, XXXIX cycle

Matilde **Rossi**, XXXIX cycle

Simone **Ventisette**, XXXIX cycle

Samuele **Baldini**, XXXIX cycle

Lapo **Querci**, XXXIX cycle

List of Partecipants

All PhD students in Chemical Sciences who presented their research projects are listed below in alphabetical order according to their PhD cycle.

XXXVII Cycle

- Acar Mert
- Aquilia Sara
- Bonechi Marco
- Bracaglia Lorenzo
- Buco Francesca
- Cabigliera Serena Benedetta
- Cappitti Alice
- Casoria Michele
- Cosottini Lucrezia
- Dali Andrea
- Fichera Michelangelo
- Gerace Alessandro
- Pacini Lorenzo
- Porcu Daniela
- Quagliata Micheal
- Sarti Chiara
- Simonini Steiner Yschtar Tecla
- Soto Bustamante Fernando
- Spena Riccardo
- Veneri Alessandro
- Verrucchi Margherita
- Vespignani Laura

XXXVIII Cycle

- Baroni Chiara
- Biffoli Fabio
- Bonaccorso Giulia
- Chiarugi Ilaria
- Cianci Chiara
- Ciuffi Benedetta
- Conti Laura
- De Santis Ilaria
- El Barkaoui Sofiane
- Fuochi Neri
- Gallorini Riccardo
- Gentilesca Pietro
- Geri Andrea
- Mancusi Francesca
- Mangini Chiara
- Mariani Elena
- Marino Margherita
- Milano Francesca
- Pappaianni Giulio
- Pavone Sara
- Quadrini Lorenzo
- Querci Leonardo
- Riccardi Mariano
- Sahu Prem Prakash
- Sforzi Laura
- Sodini Andrea
- Tacconi Leonardo
- Tino Angela Sofia
- Tordi Pietro
- Vitale Ilaria Antonia
- Zineddu Stefano

XXXIX Cycle
Agnoloni Giulia
Albanesi Marta
Baldini Samuele
Beni Alice
Bonavolontà Deborah
Brenzini Biagioni Francesco
Bracci Silvia
Campagiorni Luca
Ceccherini Valentina
Gabellini Lapo
Lulli Thomas
Mumtaz Amina
Orlandi Matteo
Pacciani Valentina
Prifti Georgia-Myrto
Querci Lapo
Rossi Matilde
Tozzetti Martina
Turchi Filippo
Ventisette Simone
Vieira Pedro Miguel Ascenso

XL Cycle
Adamo Céline
Baldi Chiara
Baranger Emmanuel
Bianchi Elisa
Bigelli Consuelo
Briganti Debora
Callozzo Sara
Carbone Mattia
Chenin Quentin
Giovani Claudia
Gobbo Mariasole
Guiggi Livia
Isidoro Lorenzo
Lunghi Irene
Mohamedzakaria-Shibinasbarveen Naufia
Montanari Francesco
Morano Alessio
Morozzi Sara
Sartini Daniele
Serventi Francesca
Sestaioni Davide
Siadohoni Shima
Zhou Zhiyi

Programme of the Symposium

Tuesday 14th January 2025

14:00	14:45	**Opening session**	*Opening speech*	
			Chair: Andrea Sodini, Samuele Baldini	
14:45	15:03	OR01	Chiara Sarti	Addressing emerging microcontaminants in wastewater: the role of advanced nature-based solutions
15:03	15:11	OR02	Matteo Orlandi	Developing and Validating a New Force Field for Cadmium Proteins via QM/MM and MD Simulations
15:11	15:23	OR03	Angela Sofia Tino	Revealing the potential of a chimaera: a peptide-peptide nucleic acid molecule designed to interact with the SARS-CoV-2 N protein
15:23	15:31	OR04	Francesco Brenzini Biagioni	Synthesis of 5-member heteroaromatics containing peptide backbones: pro and cons of structural constraints induced by amide bond surrogates
15:31	15:43	OR05	Benedetta Ciuffi	Effect of process parameters on the physical-chemical properties of hydrochar from rigid polyurethane foams
15:43	16:15		***Coffee break***	
16:15	16:33	OR06	Lorenzo Bracaglia	Relaxation-edited NMR experiments to target multidomain proteins
16:33	16:41	OR07	Valentina Pacciani	Engineering Hybrid Synthetic-Biogenic Liquid Crystalline Nanoparticles for Biomedical Applications
16:41	16:53	OR08	Laura Sforzi	Crossing aquatic systems: insights into microplastic pollution in the Mediterranean Sea
16:53	17:01	OR09	Giulia Agnoloni	Chiral Donor-Acceptor Dyads to explore the CISS Effect
17:01	17:15		***End of day one***	

9:00	9:10		**Opening of day two**	
			Chair: Yschtar Tecla Simonini Steiner, Matteo Orlandi	
9:10	9:28	OR10	Riccardo Spena	Microfluidic approach for the analysis of encapsulating agents in fabric care
9:28	9:40	OR11	Andrea Sodini	Bacteria Outer Membrane Vesicles Conjugated with MUC1 Antigen Mimetics with Increased Immune Response
9:40	9:52	OR12	Andrea Geri	Mechanistic Studies on Antitumor Gold Compounds
9:52	10:00	OR13	Valentina Ceccherini	Metal-based drugs: an insight into the development of novel antimicrobial agents
10:00	10:18	OR14	Francesca Buco	Multivalent C2-alkylated piperidines as potential modulators of the β-glucocerebrosidase enzyme activity
10:18	10:30	OR15	Giulia Bonaccorso	Pyrolysis coupled to gas chromatography for the identification and quantification of plastic polymers in environmental and food samples
10:30	11:30		***Coffee break & Poster Session***	
11:30	11:48	OR16	Lorenzo Pacini	Solid-Phase Peptide Synthesis Beyond Dimethylformamide: Production of GLP1 agonist using green binary solvent mixture.
11:48	12:00	OR17	Mariano Riccardi	Adsorption of molecular magnets on metal surfaces
12:00	12:12	OR18	Chiara Mangini	A tailored CNC-AuNPs hybrid for precision radiotherapy in oncology
12:12	12:30	OR19	Michelangelo Fichera	Production of carbonaceous materials from biomass of high environmental hazard, their characterization and application for water depuration and analytical purposes

12:30	12:38	OR20	Deborah Bonavolontà	Natural non-lamellar lipid scaffolds for cosmetics applications
12:38	12:50	OR21	Pietro Gentilesca	Development of materials for the selective coordination of critical elements present in production waters
12:50	13:02	OR22	Elena Mariani	Advancing Electroplating: The Potential of Pulsed Current Techniques for Superior and Sustainable Coatings
13:02	14:00		***Lunch***	
			Chair: Andrea Dali, Lapo Querci	
14:00	14:18	OR23	Fernando Soto Bustamante	Characterizing Viscoelastic Properties and Confinement-Induced Dynamics in PVA-Chitosan Hydrogels
14:18	14:30	OR24	Fabio Biffoli	Sustainability and optimization of an electroplating industry: from multilayer engineering to theoretical understanding of charge transfer processes
14:30	14:38	OR25	Lapo Gabellini	The use of XPS photoelectron and Auger lines in the characterization of catalysts and their supports
14:38	14:50	OR26	Neri Fuochi	Innovative Smart Materials: From Reversible Shape Control to Passive Sweat Collection in Microfluidic Sensors
14:50	15:08	OR27	Lucrezia Cosottini	Ferritin-based anticancers
15:08	15:35		***Coffee Break***	
15:35	15:53	OR28	Marco Bonechi	Oxygen Reduction Reaction Catalysts from Electroplating Industries Waste Solution
15:53	16:01	OR29	Martina Tozzetti	Biomimetic Nanoarchitectures for Aerosol Treatment

16:01	16:09	OR30	Matilde Rossi	Development of peptide nucleic acids-based molecules targeting G-quadruplex structures
16:09	16:17	OR31	Pedro Miguel Ascenso Vieira	Precision cancer therapy: strategies to selectively inhibit the biosynthesis of cancer associated glycans
16:17	16:30		***End of day two***	

9:00	9:10		**Opening of day three**	
			Chair: Leonardo Tacconi, Matilde Rossi	
9:10	9:28	OR32	Michele Casoria	Exploring Glycopeptide and Glycoprotein Structure and Dynamics. A Computational Study: from Classical Methods to Machine Learning Approaches
9:28	9:40	OR33	Chiara Baroni	Dual-Targeting Anticancer Agents: Design and Evaluation of Compounds Targeting Carbonic Anhydrase and Histone Deacetylase
9:40	9:52	OR34	Francesca Mancusi	Repurposed and novel molecules in photodynamic therapy with antimicrobial activity
9:52	10:00	OR35	Alice Beni	Wound Management: the importance of prevention and of appropriate treatments
10:00	10:18	OR36	Daniela Porcu	New strategies for the monitoring and the inhibition of metals and alloys corrosion in Cultural Heritage
10:18	10:30	OR37	Stefano Zineddu	Exploring the potential of metal-based compounds against multidrug resistant pathogens: the case of Burkholderia cenocepacia
10:30	11:30		***Coffee break & Poster Session***	
11:30	11:48	OR38	Michael Quagliata	Peptide Inhibitors of SARS-CoV-2 Cell-Entry: Synthesis, Structural Analysis, and Biological Evaluation
11:48	12:00	OR39	Laura Conti	Non-lamellar Lipid Nanoparticles as Innovative Vectors for RNA Delivery
12:00	12:12	OR40	Ilaria Chiarugi	Development and Optimization of Self-Assembling Modified Beta-Cyclodextrin-Based Nanocarriers for gene delivery
12:12	12:30	OR41	Alessandro Gerace	Synthesis of innovative nanomaterials to develop improved Rare Earths-free permanent magnets

12:30	12:38	OR42	Samuele Baldini	Development and characterization of emulsion-templated PDMS organogels for modern and contemporary artworks cleaning
12:38	12:50	OR43	Prem Prakash Sahu	Computational Exploration of Magnetic Exchange in Transition Metal Molecular Spin Qubits: From Isolated Molecules to Bulk Phases
12:50	13:02	OR44	Chiara Cianci	Sustainable Nanostructured Coatings for the Conservation of Street-Art
13:02	14:00		***Lunch***	
			Chair: Prem Prakash Sahu, Lorenzo Pacini	
14:00	14:18	OR45	Margherita Verrucchi	Electrochemical Strategies and Electrodeposition Techniques for Advancing Decorative Electroplating Applications
14:18	14:30	OR46	Leonardo Tacconi	Enhancing the rotating magnetocaloric effect in lanthanide complexes via high order magnetic anisotropies
14:30	14:38	OR47	Marta Albanesi	Ultra-low temperature magnetic investigation of a single molecule magnet on a type-II superconductor
14:38	14:50	OR48	Pietro Tordi	Multiresponsive Ionic Conductive Alginate/Gelatin Organohydrogels with Tunable Functions
14:50	15:08	OR49	Sara Aquilia	Valorization of Rapeseed Meal Proteins to Developing Sustainable Biodegradable Composites
15:08	15:35		***Coffee Break***	
15:35	15:53	OR50	Yschtar Tecla Simonini Steiner	Recognition of emerging pollutants (EPs) with artificial fluorescence chemical sensors: a supramolecular approach
15:53	16:01	OR51	Thomas Lulli	A Key Cope-House Reaction Accomplishes the First Stereoselective Synthesis of Polyhydroxylated 3-Methylindolizidines

16:01	16:09	OR52	Simone Ventisette	Synthesis and Application of Polynorepinephrine-Derived Biomimetic Receptors: Nanoparticles and Films for Advanced Biosensing
16:09	16:17	OR53	Silvia Bracci	Anti-MOG glycopeptide antibodies for MOG antibody-associated disease patient stratification
16:17	16:30		***End of day three***	

9:30	9:40		**Opening of day four**	
			Chair: Simone Ventisette, Silvia Bracci	
9:40	9:58	OR54	Alice Cappitti	Design and applications of innovative polymeric materials
9:58	10:10	OR55	Ilaria De Santis	Gold nanoparticles and lipid vesicles: a gateway to advanced nanoplasmonic and SERS probes for biomedical applications
10:10	10:18	OR56	Luca Campagiorni	Study of the physico-chemical properties and hydration reactions of cement formulation based on ground granulated blast furnace slag with varying sulfate content
10:18	10:30	OR57	Sara Pavone	Synthesis of iminosugar derivatives as potential agrochemicals for crop protection
10:30	10:42	OR58	Giulio Pappaianni	Electrodeposition and modification of surfaces of technological interest with low environmental impact
10:42	11:00	OR59	Serena Benedetta Cabigliera	Technological and biological innovations in tackling Microplastics and Microfibers Pollution
11:00	11:08	OR60	Filippo Turchi	Targeting Intrinsically Disordered Proteins in Neurodegenerative Diseases: Exploring pharmacological chaperone for Dual Action on α-Synuclein and GCase
11:08	11:30		***Coffee Break***	
11:30	11:48	OR61	Alessandro Veneri	Eco-Friendly Optoelectronic Devices: Semiconductors and Solar Cells for a Cleaner Tomorrow
11:48	12:00	OR62	Riccardo Gallorini	Comparative Evaluations of Thermochemical Reactions for Residual Biomass Conversion
12:00	12:12	OR63	Margherita Marino	Antibody-drug conjugates: a strategy of purification and identification

12:12	12:20	OR64	Lapo Querci	Development of hybrid devices based on a liquid metal alloy junction
12:20	12:38	OR65	Andrea Dali	Advanced spectroscopic study aiming to the understanding of the heme biosynthetic pathway of Gram-positive bacteria
12:38	12:46	OR66	Amina Mumtaz	Removal of PFAS by Graphene nanosheet polymer
12:46	12:58	OR67	Ilaria Antonia Vitale	Design and Development of Wearable Electrochemical Sensor for The Monitoring of Clinical Parameters
12:58	14:00		***Lunch***	
			Chair: Leonardo Tacconi, Andrea Sodini	
14:00	14:18	OR68	Mert Acar	Hofmeister Effects on the Gelation Properties of a Peptide Hydrogel
14:18	14:30	OR69	Lorenzo Quadrini	Electrochemical Urea Sensing in Wastewater Using a Flow Biocatalytic Approach
14:30	14:42	OR70	Francesca Milano	Dextran-Modified Poly(allylamine) Nanoparticles as Nanocarriers for the Delivery of Enzymes involved in Lysosomal Storage Diseases
14:42	15:00	OR71	Laura Vespignani	Study of new eco-friendly materials for Cultural Heritage preservation
15:00	15:08	OR72	Georgia-Myrto Prifti	Multivalent Golgi-targeting compounds for the precision delivery of cancer therapeutics

15:08	15:20	OR73	Leonardo Querci	Shedding light on the electron delocalization pathway at the $[Fe_2S_2]^{2+}$ cluster of FDX2
15:20	15:32	OR74	Sofiane El Barkaoui	Optimising Biochar-Based Column Filtration Systems for Enhanced Pollutant Removal in Wastewater Treatment: A Preliminary Study
15:32	16:00	***Closing session***		

List of Oral Presentations

OR01

Addressing emerging microcontaminants in wastewater: the role of advanced nature-based solutions

Chiara Sarti[a,b,c], Alessandra Cincinelli[a], Tania Martellini[a], Gabriela Dotro[b], Fabio Masi[c], and Tao Lyu[b]

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Emerging microcontaminants (EMs), including organic UV filters (OUVAs), per- and poly-fluoroalkyl substances (PFAS), and microplastics (MPs), are persistent pollutants in aquatic environments due to their inefficient removal in conventional wastewater treatment plants (WWTPs). This PhD research focuses on sustainable approaches to manage EMs in wastewater, addressing both removal strategies and analytical challenges. The study presented here, developed in collaboration with Cranfield University (UK), provides evidence of the advancements in constructed wetland (CW) technology for EM treatment and mitigation.

CWs are widely recognized for their cost-effectiveness and operational simplicity in wastewater treatment compared to conventional systems. Beyond traditional applications, CWs show potential to mitigate EMs such as MPs and PFAS. To enhance efficiency and reduce spatial footprint, this research explores innovative strategies such as replacing traditional substrates (e.g., gravel) with electroconductive (EC) media. Microbial electrochemical technology-based treatment wetlands (METlands) leverage EC materials to support electron transfer processes driven by electroactive bacteria (EABs) [1]. While METlands have demonstrated superior nutrient removal compared to conventional CWs [2], [3], their effectiveness in addressing EMs remains underexplored. This study investigates the occurrence, characteristics, and removal efficiency of MPs and PFAS in two pilot-scale METland systems treating raw sewage and primary treatment effluents. The performance of METlands is compared to conventional gravel-based CWs to assess the impact of substrate type on EM removal. Results indicate that EC media enhance MPs and PFAS removal, potentially due to improved physical adsorption and chemical interactions with the substrate.

Optimization of substrate materials in CWs represents a critical step toward advancing nature-based solutions for EM mitigation. By integrating innovative materials and approaches, CWs can play a pivotal role in reducing MP and PFAS pollution, contributing to the restoration of aquatic environments, and promoting ecosystem health.

[1] C. A. Ramírez-Vargaset al., *Sci. Total Environ.* **2019**, *659,* 796–806.
[2] A. Aguirre-Sierra et al., *Environ. Sci.: Water Res. Technol.* **2020**, *6*, 1312-1323.
[3] A. Prado et al., *Sci. Total Environ.* **2020**, *735*, 139522.

OR02

Developing and Validating a New Force Field for Cadmium Proteins via QM/MM and MD Simulations

Matteo Orlandi[a,b], Marina Macchiagodena[a] , Piero Procacci[a], Fabrizio Carta[b], Claudiu T. Supuran[b], and Marco Pagliai[a]

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Understanding the polarization effect induced by transition metals on proteins during classical molecular dynamics (MD) simulations is a crucial challenge in computational chemistry. Our research project led us to develop a new Force Field (FF) tailored for metallic cofactors in biomolecules, specifically focusing on Cadmium (II) binding proteins. MD simulations, a class of computational chemistry methods, allow us to describe molecular systems by treating particles classically. By integrating the Newtonian equations of motion for every atom, MD simulations enable us to study the time evolution of molecular systems deterministically. Relying on classical mechanics, the intramolecular and intermolecular interactions are described by potential energy terms represented by a Force Field. Our upgraded FF for Cadmium proteins captures the polarization of coordinating residues, closely reproduces experimental distances and maintains the tetrahedral coordination pattern. Moreover, we employed MD simulations with a QM/MM approach as a high-level validation tool for our newly developed Force Field. While evidence has accumulated over the years regarding cadmium toxicity in living organisms, the mechanism by which this ion exerts its toxic effects on proteins remains unclear. Our FF might help shed light on the origins of Cd-induced bio-aberrations at the molecular level, in combination with experimental evidence.[1]

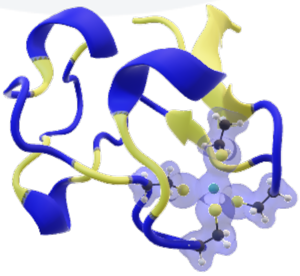

Figure 1: Electron density of the QM subsystem in the 1R0I protein.

[1] M. Macchiagodena et al., *JCIM* **2019** *59* (9), 3803-3816.

OR03

Revealing the potential of a chimaera: a peptide-peptide nucleic acid molecule designed to interact with the SARS-CoV-2 N protein

Angela S. Tino[a,b,c], Michael Quagliata[a,c], Marco Schiavina[a,b], Lorenzo Pacini[a,c], Anna Maria Papini[a,c], Isabella C. Felli[a,b], and Roberta Pierattelli[a,b]

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[b]Magnetic Resonance Center, Via L. Sacconi 6, 50019-Sesto Fiorentino, Florence, Italy
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Numerous RNA-binding proteins have modular structures with folded domains and intrinsically disordered regions, making their atomic characterization difficult. This severely limits the investigation of their modalities of interaction as well as the evaluation of possible ways to interfere with this process. We report herein a rational strategy for the design and synthesis of a ligand able to interfere with the protein function, monitoring the interaction through solution nuclear magnetic resonance spectroscopy. Our approach employs a chimaera composed of two different fragments, a peptide and a peptide-nucleic acid, allowing to incorporate in the resulting molecule key features to address RNA-protein interactions. Focusing on two constructs of the N protein from SARS-CoV-2, the globular N-terminal domain and a more extended one comprising also two flanking intrinsically disordered regions, we demonstrate the enhanced affinity of the designed peptide-peptide nucleic acid chimaera for the protein compared to a related peptide lacking π-π stacking contributions within the chain. Furthermore, we emphasize the increasingly recognized relevant and synergistic role of the intrinsically disordered regions in protein-ligand interaction.[1,2]

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[1] L. Pontoriero et al., *Biomolecules*, **2022**, *12*, 1.
[2] R. Sekine et al., *J. Biochem*. **2023**, *173*, 6.

OR04

Synthesis of 5-member heteroaromatics containing peptide backbones: pro and cons of structural constraints induced by amide bond surrogates

Francesco Brenzini Biagioni[a,b], Karine Porte[a], Pierre-Yves Renard[a], and Anna Maria Papini[b]

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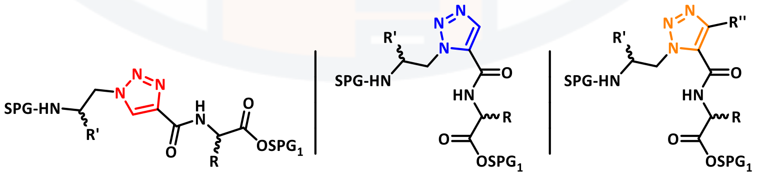
Increasing the stability and bioavailability of short peptides *in vivo* is fundamental for the development of peptide-based drugs. The main challenges to address are the low metabolic stability and the high conformational flexibility of peptides, that can lead to inactivation and decrease of their activity. To avoid these issues, one strategy is the use of peptidomimetics, in which the peptide bond is replaced by analogues with similar properties. The introduction of heteroaromatic cores into the peptide backbone improves the metabolic stability and also increases the structural constraints, providing an interesting and promising class of mimetic molecules.[1] This work is aimed to the development of peptidomimetics using regioselective metal catalyzed 1,3-dipolar cycloadditions, in order to offer either s-*cis* or s-*trans* peptide bond mimetics. The focus is mainly on the 1,4- and 1,5- disubstituted 1,2,3 triazoles, which present structural features similar to the peptide bond and a low toxicity.[2] In addition, the concept of peptidomimetics will be extended by developing mimetics able to mimic both the peptide bond and an amino acid, through the introduction of the 1,4,5- trisubstituted 1,2,3 triazole. Final aim is to investigate the biological properties of new analogues modulating the accuracy of the mimetics, as well as impact on serum stability versus the side-chain to side-chain triazolyl bridged peptides.[3]



1,4 triazonyl dipeptide **1,5** triazonyl dipeptide **1,4,5** triazonyl dipeptide

Figure 1: The proposed triazolyl dipeptides, which will be introduced into peptide sequences as mimetics of the peptide bond, and in case of trisubstitution, of an amino acid. SPG: semi-permanent protecting group.

[1] I. Cerminara *et al.*, *Pharmaceuticals* **2012**, *5(3)1*, 297-316.
[2] P. Bruyat *et al.*, *J. Org. Chem.* **2018**, *83(21)*, 13515-13522.
[3] F. Nuti *et al.*, *J. Enzyme inhib. Med. Chem.* **2023**, *38(1)*, 2254019.

OR05

Effect of process parameters on the physical-chemical properties of hydrochar from rigid polyurethane foams

Benedetta Ciuffi[a], Emiliano Fratini[a,b], G. Ferraro[a,b], and Luca Rosi[a]

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Polyurethane (PUs) are one of the high consumption commodity polymers, and their production in Europe has reached 3.6 Mt, a value comparable to that of other commercial polymers such as PET and PVC.[1] Among the main applications of PUs, rigid foams (PUR) are one of the prominent products. Due to their high rate of production and usage, million tons of PUR waste are produced every year and sent to landfill.[2] Recycling is a great alternative to landfilling, but it is still not a predominant method of PUR waste disposal, mainly due to the thermosetting nature of PUR. In this work, the thermochemical recycling of PUR was evaluated through hydrothermal liquefaction (HTL) and hydrothermal carbonization (HTC) with the aim of producing a solid carbon-based material, called *hydrochar* (HC), as high added-value product. Reactions were carried out using a Parr reactor 4576 HP and ultrapure water in subcritical conditions. During this study it was evaluated how the process parameters (temperature, T; residence times, t_r; feedstock/solvent ratio, f/s), can influence the yield of HC and its physical-chemical properties. Moreover, for the first time in literature an acidic environment was experimented, using a mixture of water and acetic acid (pH=2,06). As expected from literature,[3] an increase in T (from 250 °C to 345 °C) causes a drastic decrease in the HC yield, vice versa a significant increase in the f/s (from 0.02 to 0.06) causes an increase in the HC yield. The f/s has also an effect on surface porosity formation. Working at high dilution (f/s=0.02), the formation of pores in the order of hundreds of nm is observed. All the produced HCs show a high calorific value, major than that of PUR itself (27.6 MJ/Kg), this is indicative of energy densification process and suggest their possible use as solid fuels.

[1] Plastics Europe, https://plasticseurope.org/knowledge-hub/the-circular-economy-for-plastics-a-european-analysis-2024/.
[2] A. Kemona et al., *Polymers.* **2020,** *12*, 1752.
[3] C. Oktaviananda et al., *AIP Conf. Proc*. **2017,** *1823 (1)*, 020029.

OR06

Relaxation-edited NMR experiments to target multidomain proteins

Lorenzo Bracaglia, Silvia Oliveti, Isabella C. Felli, and Roberta Pierattelli

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CREB-binding protein (CBP) functions as a transcriptional coactivator, playing a critical role in the regulation of numerous human genes and signaling pathways [1]. CBP consists of a combination of largely disordered regions and seven structured globular domains. Traditional structural characterization of CBP has predominantly focused on isolated domains, facilitating the application of techniques like NMR spectroscopy and X-ray crystallography, but limiting the insights to single domains. This study introduces an alternative strategy that utilizes NMR spectroscopy to investigate a CBP construct encompassing two contiguous regions: the globular zinc-binding TAZ2 domain [2] and the adjacent intrinsically disordered ID4 region [3]. Tailored two- and three-dimensional NMR experiments were employed to enhance spectral quality, leveraging the differing structural and dynamic properties of the two domains. Our findings reveal that the structural features of TAZ2 and ID4 are mutually influenced by their interaction. Structural predictions of the multidomain construct are also presented to visualize the conformational space sampled by the construct. This work broadens the application of NMR techniques to multidomain systems, providing deeper insights into the interplay between ordered and disordered protein regions. The data presented were submitted for publication.

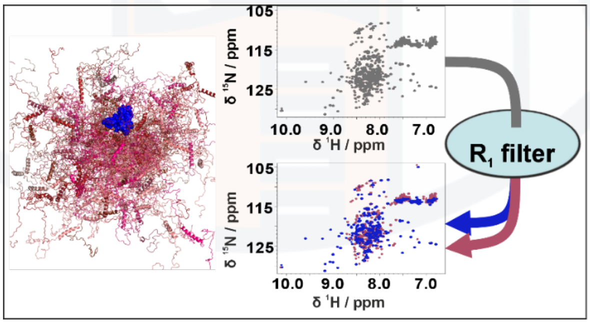

Figure 1: On the leftmost part of the panel 100 randomly generated TAZ4 conformers are shown. On the rightmost part of the panel the filtering strategy is sketched. The peaks in a standard 2D HN spectrum (grey) can be selectively tagged using a longitudinal relaxation filter. Thus, it is possible to distinguish the peaks deriving from the globular domain (blue), from those deriving from the disordered region (red).

[1] H. J. Dyson and P. E. Wright, *J. Biol. Chem.* **2016,** *291*, 6714-6722.
[2] R. N. De Guzman et al., *J. Mol. Biol.*, **2000**, *303(2)*, 243-253.
[3]. A. Piai et al., *Biophys. J.* **2016**, *110(2)*, 372-381.

OR07

Engineering Hybrid Synthetic-Biogenic Liquid Crystalline Nanoparticles for Biomedical Applications

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Extracellular vesicles (EVs) are naturally occurring particles secreted by most cells. Their intrinsic tissue-targeting and immune-evasive properties make them attractive candidates for drug delivery. However, their practical application is hindered by challenges in scalability, cargo loading efficiency, and structural stability.[1] One promising strategy to address these limitations involves merging natural EVs with synthetic drug delivery vectors to obtain hybrid nanoparticles. In this study, we present a novel approach for hybridizing EVs with lipid liquid crystalline nanoparticles (LCNPs). Unlike traditional lipid vesicles, LCNPs feature a non-lamellar structure with a high surface area-to-volume ratio, offering enhanced cargo loading, containment, and protection, as well as improved fusogenic properties.[2,3] Using a microfluidic protocol, we engineered hybrid nanoparticles by integrating red blood cell-derived EVs (RBCEVs) with cubosomes composed of the synthetic lipid glycerol monooleate (GMO). This approach produced colloidally stable hybrid LCNPs without employing polymeric steric stabilizers, thereby preserving the bioactive surface functionality of EVs. Structural and morphological analyses, including Small Angle X-ray Scattering (SAXS) and Cryo-Transmission Electron Microscopy (Cryo-TEM), confirmed the effective incorporation of EV components into the GMO matrix. In summary, these findings contribute to the development of hybrid synthetic-biogenic nanoparticles as versatile drug-delivery vectors, offering potential improvements in targeting precision, cargo loading efficiency, and therapeutic performance.

Figure 1: Scheme of the microfluidic protocol employed for the synthesis of hybrid biogenic-synthetic cubosomes

[1] I.K. Herrmann et al., *Nat. Nanotechnol.* **2021**, *16*, 748–759.
[2] H.M.G. Barriga et al., *Angewandte Chemie International Edition* **2019**, *58*, 2958–2978.
[3] A. Balestri et al., *Colloids Surf B Biointerfaces* **2023**, *231*, 13532.

OR08

Crossing aquatic systems: insights into microplastic pollution in the Mediterranean Sea

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This study is in line with the activities of the project RETURN - multi-Risk sciEnce for resilienT commUnities undeR a changiNg climate project, in the framework of the National Recovery and Resilience Plan (PNRR), Mission 4, Component 2 "From Research to Enterprise", funded by the European Union NextGenerationEU. In collaboration with the Department of Biology of the University of Florence, this research aimed to assess the presence of microplastics (MPs) in the Mediterranean Sea through the analysis of surface water and mud mullet (Mullus barbatus) samples. MP pollution in aquatic systems has emerged as an urgent environmental issue with significant implications for human health.[1] This is the first study to report results from multiple sites in the entire Mediterranean basin within the same sampling campaign and within a limited time period. Water samples were filtered directly, while mullet samples were pre-treated with an oxidative (H_2O_2) and alkaline digestion (NaOH), to remove most of the inorganic matter. The samples were then filtered, and MPs were detected and classified using stereomicroscopy and microFTIR spectroscopy. The results showed an average concentration of 70.7 items/L in the waters and 15.2 items/g ww in the mullets. The most abundant colors were black, red, and blue, and fibers represented the most frequent morphology. Cellulose, PP, PET and PE were the most detected polymers in each matrix. Data on MPs concentrations in mullet samples were used to calculate the number of MPs ingested daily by different categories (adults, children and pregnant women),[2] showing that seafood ingestion should be considered a vector of major concern for human exposure to MPs. Finally, the absence of analysis protocols for MPs in food, whose matrix complexity often leads to challenges in sample processing, is critical.

[1] T. Sun et al., *J. Hazard. Mater*. **2022**, *424,* 127533.
[2] EFSA, *EFSA Journal,* **2016**, *14(6)*, e04501.

OR09

Chiral Donor-Acceptor Dyads to explore the CISS Effect

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This research project is focused on the design, synthesis, resolution, and characterization of chiral donor-acceptor dyads, to explore the Chirality-Induced Spin Selectivity (CISS) Effect.[1] The acceptor, a perylene diimide (red portion in Figure 1), is covalently linked through bridges of various structure and length (green portion in Figure 1) to a chiral donor unit consist in a thia-bridged triarylamine hetero[4]helicene (blue portion in Figure 1).[2] The single enantiomer of each donor-acceptor dyad has been obtained through chiral HPLC, and the interaction with circularly polarized light, as well as the electronic properties of all single enantiomers investigated. The goal of this research project is to investigate the CISS effect during photoinduced electron transfer processes from the chiral donor to the acceptor, through time-resolved electron paramagnetic resonance spectroscopy (tr-EPR). Understanding this effect at the intramolecular level paves the way to design new chiral organic devices with potential applications in the field of quantum information science.[3]

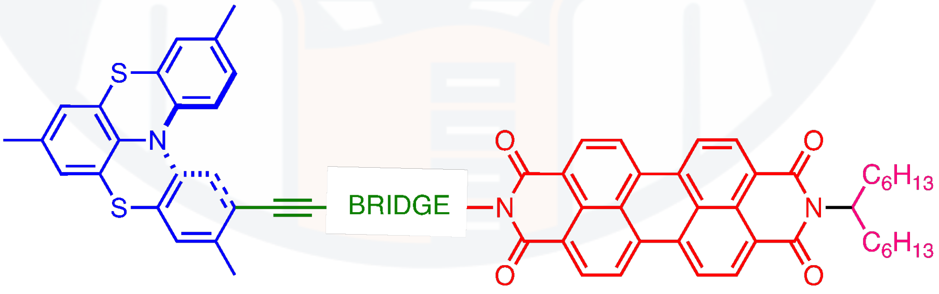

Figure 1: Chiral donor-acceptor dyads.

[1] R. Naaman et al., *Nat. Rev. Chem.* **2019**, *3*, 250-260.
[2] C. Viglianisi et al., *Chem. Commun.*, **2015**, **51**, 11452-11454.
[3] R.Sessoli et al., *Adv. Mater.* **2023**, *35*, 2300472.

Acknowledgements: We acknowledge the support of the European Union by the Next Generation EU project B12B23000300006 "Progettazione, sintesi e studio di sistemi chirali a selettività di spin nel trasferimento elettronico per il controllo di spin qubit molecolari". We also acknowledge the support from the Horizon Europe Programme through ERC-Synergy project CASTLE (proj. n. 101071533).

OR10

Microfluidic approach for the analysis of encapsulating agents in fabric care

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Encapsulation is a key strategy for efficient delivery of active ingredients. Currently, the performance of capsules in fabric care products is tested using washing machines, which consume significant amounts of water and energy. Furthermore, this method does not allow for real time analysis, requiring additional testing approaches. This study aimed to design and develop a system to replace or complement traditional methods, not only replicating results but also providing deeper insights into encapsulant-fabric interactions.

Specifically, this research project proposes a micro- and millifluidics approach, such as a 'washing machine on a chip', with the aim of both replacing standard washing machine tests with a more environmentally friendly methodology and providing 'live' information, thus significantly improving the current analytical tools used by companies. In this case, two types of devices have been designed and manufactured with the possibility of inserting a content, i.e. a small piece of fabric. Depending on the geometry selected, the sample containing a capsule dispersion can flow in different orientations, within the chip, interacting differently with the tissue in a tangential or orthogonal manner. In addition, the devices can be used to monitor the interaction over short and long periods of time by using a cover glass at the bottom. This provides access to qualitative and quantitative information on the interaction of capsules with fabrics at different time scales. Overall, a remarkable accordance between the results obtained *via* standard washing machine tests and *via* washing-machine-on-a-chip was highlighted, showing that the developed devices are good candidates for replacing washing machine tests for evaluating the efficiency of encapsulant formulations. Moreover, live visualization through confocal microscopy on fluorescently labelled capsules interacting with fabrics allowed gaining mechanistic information on capsules-fabrics interaction pathway. This suggests that the system may be a promising tool for disentangling the mechanistic details of capsule-fabric interaction, representing a promising approach to be employed for the study of current, but also future developed, encapsulating agents.

OR11

Bacteria Outer Membrane Vesicles Conjugated with MUC1 Antigen Mimetics with Increased Immune Response

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Carbohydrate-based therapeutic vaccines are forefront as targeted immunotherapies for cancer treatment. Aberrant glycosylation plays, indeed, a crucial role in tumor biology by creating "neo-epitopes," known as tumor-associated carbohydrate antigens (TACAs), which are vital for cancer initiation, progression, and metastasis. Among these, mucin-type O-glycans Tn and STn are established targets for cancer vaccine development. In this frame, we took advantage from engineered Outer Membrane Vesicles (OMVs), as a platform for vaccine formulation to present glycan antigens. OMVs were modified to display multiple copies of structurally locked Tn or STn mimetics as prototypes for cancer vaccines (**Figure 1**). The non-adjuvanted formulations, so obtained, showed strong immunogenicity *in vivo* and remarkable efficacy in a mouse model of aggressive triple-negative breast cancer.[1,2]

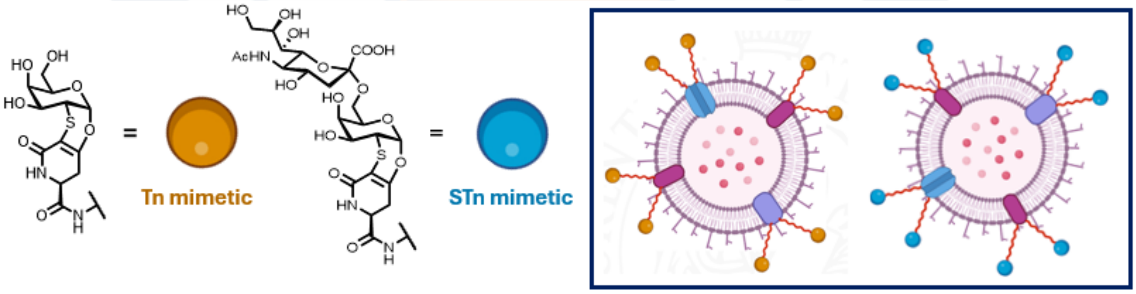

Figure 1: Tn mimetic, STn mimetic and glycosylated OMVs.

[1] E. Pesce et al., *submitted.* **2024**.
[2] N. Berois et al., *Cancers (Basel)*, **2022**, *14*, 645.

OR12

Mechanistic Studies on Antitumor Gold Compounds

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Owing to the great success of Pt-based drugs in anticancer chemotherapy, the study of gold complexes has gained a lot of interest in view of the discovery of innovative antitumor agents. While Pt drugs exert their actions mainly through binding to genomic DNA and nucleic acids, the main targets of anticancer Au complexes are proteins, typically interacting with the gold center through specific thiol/selenol residues. However, the precise modes of action of gold compounds remain largely unexplored.

During my PhD, several ESI-MS binding studies have been conducted according to a well-established experimental protocol developed in our laboratory. Several different experimental conditions were tested to obtain detailed information on the binding mode between selected Au compounds and different model and target proteins.[1,2]

Generally, the analysis of the obtained mass spectra revealed the formation of stable adducts, especially with human thioredoxin reductase (hTrxR), which is considered one of the primary targets of the gold drugs. In addition, a liquid chromatography-mass spectrometry (LC-MS) methodology was developed and optimized for the analysis of gold-protein adducts. This method involves proteolytic digestion with trypsin, followed by peptide mapping and mass spectrometric analysis to determine the specific binding sites of gold complexes on the protein. Initial experiments with ferritin confirmed cysteine residues as the primary binding sites for gold complexes.[3] Furthermore, a comprehensive proteomic study was conducted on A2780 ovarian cancer cells treated with gold complexes. Quantitative proteomic analysis revealed distinct perturbations in cellular pathways, highlighting mechanistic difference among the compounds.

Overall, these studies strongly support the view that the selenol-thiol group is the true anchoring site for gold compounds in proteins and set the stage to better understand their mechanism of action. Future work will include extending the LC-MS method to additional targets, such as hTrxR, and biochemical validations will be performed, providing a more comprehensive understanding of the molecular mechanisms underlying the action of gold-based complexes.

[1] A. Geri e al., *Molecules*. **2023**, *28 (13)*, 5196.
[2] A. Geri et al., *ChemPlusChem*., **2024**, *89 (2)*, e202300321.
[3] L. Cosottini et al., *Angew. Chem.* **2024**, *63 (40)*, e202410791.

OR13

Metal-based drugs: an insight into the development of novel antimicrobial agents

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Antimicrobial resistance represents a serious risk to public health systems and there is an urgent need to find alternatives to the current antimicrobial agents. Considering this, transition metal complexes are attractive candidates for the development of new antibacterial agents due to their structural diversity, ligand exchange capabilities, and redox and catalytic properties. All these factors enable different mechanisms of action, from the ability of the metal moiety to form covalent or non-covalent bonds with biological targets, to their capability to promote photochemical processes upon light irradiation, such as ROS production or the release of active ligands.[1] In this presentation, we focus on the exploration of the potential of some metal complexes, designed to combine multiple reactivities, to act as antibacterials. In particular, a Ru-Au heterobimetallic series of complexes was conceived by merging Ru(II)-polypyridyl systems with Au(I)-N-heterocyclic carbenes. Ru(II)-polypyridyl complexes exhibit particular antibacterial properties through interactions with biological substrates and are considered appropriate photosensitizers for Antimicrobial Photodynamic Therapy and for the photoinduced release of bioactive species in Photorelease Antibacterial Therapy.[2] Au(I)-N-heterocyclic carbene complexes are also recognized for their potential antibacterial activity, primarily by inhibiting thioredoxin reductase, an enzyme implicated in the redox balance of bacteria.[3] On these bases, our goal was to leverage the different mechanisms of action and targets of these two components to develop compounds with dual activity, which could potentially be activated by controlled photosubstitution. Moreover, in light of the promising properties of Ru(II)-polypyridyl complexes, a series of highly positively charged dinuclear Ru(II)-polypyridyl systems was designed. In fact, many structurally similar complexes have demonstrated remarkable antibacterial activity and intriguing mechanisms of action, often attributed to their ability to disrupt bacterial membranes prior to internalization and their selective targeting of bacterial cells over eukaryotic ones.[2]

[1] T. Gianferrara et al., *Dalton Trans.* **2009**, *37*, 7588-7598.
[2] F. Li et al., *Chem. Soc. Rev.* **2015**, *44(8)*, 2529-2542.
[3] Y. Liu et al., *Drug Discov. Today* **2022**, *27(7)*,1961-1973.

OR14

Multivalent C2-alkylated piperidines as potential modulators of the β-glucocerebrosidase enzyme activity

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The enzyme β-glucocerebrosidase (GCase) is a lysosomal glycosidase whose misfolding is linked to the rare lysosomal storage disorder known as Gaucher Disease. One way to restore GCase activity is through Pharmacological Chaperones (PCs), molecules able to bind and stabilize misfolded GCase resulting in enzyme activity's enhancement [1]. Iminosugars (i.e. carbohydrates analogues with a nitrogen atom replacing the endocyclic oxygen) such as the *2*-octyl 3,4,5-trihydroxypiperidine **1** are promising PCs for GCase [2] (Figure 1). In addition, multivalency has proven to be a highly effective strategy for modulating GCase activity and the multimerization of iminosugars in different scaffolds have been reported [3]. However, multivalent systems based on compound **1** are not present in the literature. This project is focused on the multimerization of a *C2*-alkylated 3,4,5-trihydroxypiperidine onto dendrimers and gold nanoparticles (AuNPs) (Figure 1). The azido-functionalized piperidine **2** has been chosen as key intermediate for copper-catalyzed alkyne-azide cycloaddition (CuAAC) reactions with the alkyne-bearing scaffolds **4a–c** or propargylated thiol-ending linker suitable for further grafting onto AuNPs. The *in vitro* modulation of GCase activity by these multivalent systems has been studied.

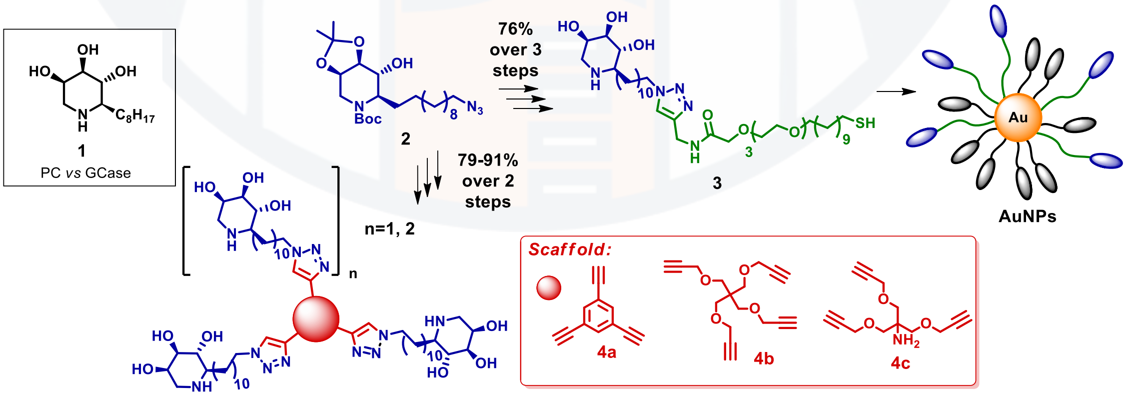

Figure 1 Lead PC compound **1** alongside newly developed multivalent iminosugars

[1] D. M. Pereira et al., *Chem. Sci.* **2018**, *9*, 1740-1752.
[2] F. Clemente et al., *Bioorg. Chem*. **2020**, *98*, 103740.
[3] M. Martìnez-Bailén et al., *Pharmaceuticals* **2022**, *15*, 823.

OR15

Pyrolysis coupled to gas chromatography for the identification and quantification of plastic polymers in environmental and food samples

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In this study, a method for the analysis of microplastics in environmental and food matrices was developed using pyrolysis coupled to gas chromatography-mass spectrometry (Py-GC-MS). The occurrence of microplastics in environmental matrices is an issue becoming increasingly important, requiring the development and optimization of reliable analytical methods for their quantification. In this regard, there is a lack of analytical methods capable of analyzing microplastics capable to express their concentrations (e.g., µg/L and/or µg/g), as it is commonly done for all micropollutants. Py-GC-MS technique, which has this advantage,[1] was therefore used for the identification and/or quantification of 8 microplastics (PMMA, PS, PET, PP, PE, PVC, PC and PA 6,6) in water samples of varying complexity. After a preliminary investigation in *full scan* mode, the method was developed in *single ion monitoring* mode, programming the acquisition windows in relation to the retention times of the pyrolysis fragments of the target polymers. Samples fortified with polymer mixtures were prepared in three types of water, i.e. demineralized water, tap water and wastewater, to optimize the filtration procedure and evaluate the recovery. Due to its complexity, wastewater was microwave digested, using hydrogen peroxide as reagent, at 75 °C, for 20 min. Eight real samples (demineralized water, tap water, bottled mineral water, fountain water and wastewater collected from four points of a wastewater treatment plant) were analyzed.

PE was quantified in all samples (1.82 - 4179 µg/L), PS in wastewater (71.5 and 20.5 µg/L) and together with PP also in bottled mineral water (0.16 and 3.42 µg/L) and fountain water (3.15 and 58.2 µg/L). PVC was also identified in all matrices except bottled mineral water, while PC was found only in fountain water and wastewater and PA only in wastewater.

[1] Y. Xu et al., *Environmental Science & Technology* **2022**, *56*, 4988-4997.

OR16

Solid-Phase Peptide Synthesis Beyond Dimethylformamide: Production of GLP1 agonist using green binary solvent mixture.

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In recent decades, the global market for therapeutic peptides has grown substantially, driven by advancements in research and technology for peptide synthesis.

The growing demand for peptide APIs at an industrial scale highlights the need for efficient, scalable, and environmentally sustainable manufacturing processes.

Solid-phase peptide synthesis (SPPS) remains the preferred strategy for medium-length peptides due to its efficiency, scalability, and automation capabilities. However, traditional SPPS depends heavily on harmful solvents like DMF, NMP, and CH_2Cl_2, raising environmental concerns. Recent research has prioritized greener solvents, efficient methods, and advanced technologies to address these challenges.[1] We utilized the PurePep Chorus synthesizer (Gyros Protein Technologies) to explore sustainable solutions. By employing magnetic induction heating and customizable reagent lines, we optimized synthesis protocols using binary solvent mixtures without DMF. These solvents, tested on model peptides such as ACP and poly-Alanine, demonstrated the feasibility of green synthesis by reducing by-products and improving process efficiency. The approach was further validated with complex peptides, comparing green solvents to traditional methods. To enhance sustainability, we implemented a catch-and-release purification method, eliminating chromatography and reducing waste.[2] Additionally, two green strategies were developed for producing Liraglutide, a GLP-1 agonist, using binary mixtures and catch-and-release for purification and acylation.[3] By bridging academia and industry, these innovations advance scalable GMP production and demonstrate a commitment to sustainability, reducing the environmental impact of peptide manufacturing.

[1] O. Al Musaimi et al., *Green Chem.* **2020**, *22.4*, 996-1018.
[2] L. Pacini et al., *J. Pept. Sci*. **2024**, *e3605*.
[3] L. Pacini et al., in preparation.

OR17

Adsorpion of molecular magnets on metal surfaces

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Molecular magnets are a promising class of materials with potential applications in spintronics, quantum computing, and data storage due to their unique magnetic and electronic properties. This study investigates the adsorption behavior of molecular magnets on metallic surfaces using a computational protocol that employs a Steele-type potential to model surface interactions efficiently. The approach balances computational cost and accuracy, enabling the examination of extended systems with molecular magnets. The potential developed captures the essential features of molecule-surface interactions while significantly reducing computational costs. The calculated structural and spectral properties are consistent with experimental findings,[1-3] validating the method's reliability for studying these types of systems.

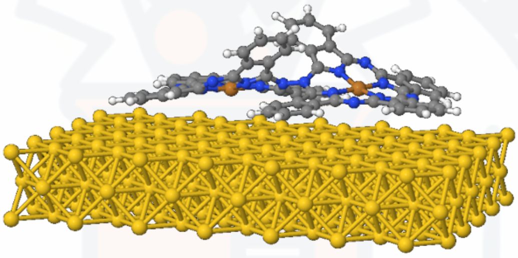

Figure 1: Copper Phthalocyanine dimer adsorbed on a gold surface.

[1] J. M. Auerhammer et al., *Surface science* **2002**, *506.3*, 333-338.
[2] M. Kothe et al., *Langmuir,* **2019**, *35.42*, 13570-13577.
[3] S. Rejaul et al., *MSDE*, **2019**, *4.3,* 471-483.

OR18

A tailored CNC-AuNPs hybrid for precision radiotherapy in oncology

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The development of nanomaterials for precision cancer therapy is a highly sought-after goal. Their custom functionalization can result in innovative tools with enhanced therapeutic efficacy and reduced side effects. However, the creation of reliable and customizable materials remains a significant challenge.[1] In this context, our research group recently developed a robust synthetic strategy to produce a hybrid glyconanomaterial that consists of cellulose nanocrystals and gold nanoparticles (CNC-AuNPs).[2] It combines the biocompatibility, biodegradability, and extended blood circulation lifetime of CNC with the radiosensitizing properties of AuNPs. Its surface can be easily engineered with high batch-to-batch reproducibility including various bioactive headgroups by subsequential copper-catalyzed azide-alkyne cycloadditions on the terminal alkyne of a lipoamide spacer on AuNPs surface and orthogonal chemistry on the hydroxyl groups of the CNC.[2] This communication describes the functionalization of CNC-AuNPs with glucose heads to yield a glyconanomaterial[3] suitable for precision radiotherapy by targeting GLUT channels. The collaboration with a multidisciplinary network[3] of collaborators allowed us to investigate the potential of the glyconanomaterial as a precision radiosensitizer for solid tumors treatment.

[1] J. Park, et al.; *Theranostics*, **2019**, *9*, 8073-8090.
[2] a) Patent WO 2023/233281 A1; b) D. B. Chithrani et al.; *Radiat Res.*, **2010** Jun,*173(6)*, 719-28.
[3] a) G. Biagiotti et al., *Nanoscale Horiz.,* **2023***, 8, 776–782*; b) G. Biagiotti et al., *Nanoscale Horiz.*, **2024**, *9*, 1211-1218.

OR19

Production of carbonaceous materials from biomass of high environmental hazard, their characterization and application for water depuration and analytical purposes

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The research aimed to produce carbonaceous materials (i.e. biochars) by thermal conversion of biological sludge from wastewater treatment plants (WWTPs) in domestic or mixed domestic-industrial contexts, which represents a waste of high environmental concern (see Figure 1). Biochars underwent to chemical and/or thermal activation processes to increase their adsorption capacity towards organic micropollutants (OMPs) of environmental concern.[1] The materials were characterized both from product (e.g. surface area, porosity distribution, etc.) and environmental viewpoints (evaluation of the release of polycyclic aromatic hydrocarbons, metals, etc.) and compared with the characteristics of reference materials, such as commercial activated carbon. The most promising materials were studied for the removal of OMPs such as pharmaceutical compound and dyes, both by kinetic tests and adsorption isotherms. Long-term tests were conducted through the implementation of biochar in constructed wetlands to evaluate the effectiveness of the biochar medium for practical applications. Best-performing materials in terms of composition and chemical release were also tested for analytical purposes (i) as sorbent for dispersive solid phase extraction (d-SPE) of QuEChERS extracts and (ii) development of carbon-based sensors.

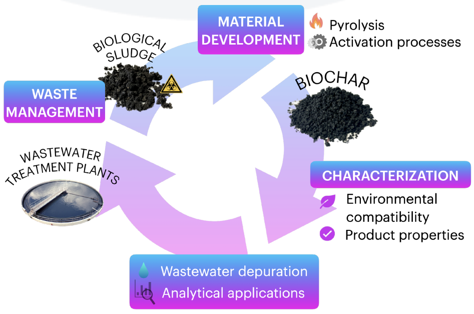

Figure 1: Circular approach to sewage sludge management and reuse in WWTPs

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OR20

Natural non-lamellar lipid scaffolds for cosmetics applications

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Lipid-based nanosystems are emerging as key platforms for delivering active ingredients in various applications, including cosmetics, due to their unique properties such as biocompatibility, structural tunability, and ease of functionalization. Among lipid assemblies, inverse lyotropic liquid crystalline (LLC) mesophases are particularly noteworthy for their high fusogenicity, large interfacial area, and ability to encapsulate both hydrophobic and hydrophilic molecules.[1,2] This study explores novel lipid formulations, derived from synthetic or natural lipids, that form LLC mesophases, aiming at developing biocompatible and efficient nanovectors. Preliminary results demonstrate the formation of ordered structures and the successful incorporation of hydrophobic active ingredients, that are derived from plants such as avocado and goji berry. Efficiency tests, including Confocal Laser Scanning Microscopy (CLSM) on Supported Lipid Bilayers (SLB) and synthetic skin models, show that these formulations can interact effectively with these interfaces under both static and dynamic conditions (Figure 1). Overall, this study will contribute to the development of complex lipid formulations based on natural lipids for cosmetics applications and to estimate their efficiency and ability to interact with bio-relevant membranes.

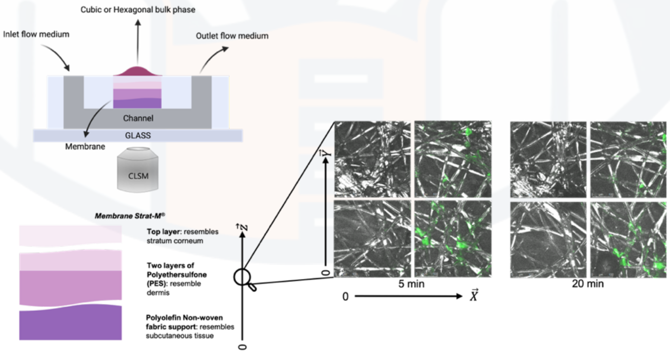

Figure 1: Illustration of a synthetic tissue modeling skin that is inserted in a millifluidic chip. The images CLSM show the spreading of the lipid LLC phase (labelled with a green fluorescent dye) with the membrane (shown in grey in the transmission image).

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OR21

Development of materials for the selective coordination of critical elements present in production waters

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Our time is characterized by an unprecedented ecological crisis. Rising temperatures around the world, extreme weather events in areas where they have never occurred before, increasing desertification in previously green areas are manifestations of this crisis. Knowing this, the sustainable management of important resources has never been more critical. One often overlooked opportunity is production waters, a salty by-product generated during oil and gas production. Due to their high salt content, these waters can contain valuable critical elements important to various industries. To date the main method used to recover these ions are unusable for temporal reasons (the processes are too long) or economic reasons (the processes are too expensive). The recovery of these ions by using selective ligands could solve these problems. Moving from the results of the last year, during the second year of the PhD we have synthesized two new generations of ligands for the recovery of Li^+ from production water. These new generations differ from the previous one (generation 1) for the presence of an aromatic group (generation 2) or greater dimensions of the binding cage (generation 3). The new ligands were characterized by mass analysis, H^1 NMR spectra and potentiometric measures. Their ability to bind Li^+ was also studied. The results show a significant improvement compared to those obtained previously. We have now extended the project to the selective recovery and valorisation of Pd(II) from wastewater. Pd(II) recovery was achieved by in situ formation of heterogeneous catalysts for the electrochemical oxygen reduction reaction (ORR) occurring at the cathode of fuel cells. Typically, ORR is catalyzed by solid Pt metal electrodes, but we have shown that cheaper atomically precise catalysts containing low Pd(II) loadings have similar efficiency.[1] New Pd(II)-based catalysts have been prepared and are being studied. Both the ligands for Li^+ recovery and the Pd(II)-based catalysts will be anchored, respectively, on activated carbon and on multiwalled carbon nanotubes (MWCNT) by spontaneous adsorption at room temperature, in water and without protective atmosphere. The material thus obtained will then be characterized and studied.

[1] P. Gentilesca et al., *Dalton Trans.*, **2024**, *53 (6)*, 2487-2500.

OR22

Advancing Electroplating: The Potential of Pulsed Current Techniques for Superior and Sustainable Coatings

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In modern galvanic industries, direct current (DC) electroplating remains the dominant method. However, the introduction of innovative approaches such as unipolar and bipolar pulse plating, made possible by advancements in electronics, offers exciting new opportunities. Despite challenges in theoretical modeling and technical implementation, pulsed current electroplating has gained traction due to its ability to influence electro-crystallization mechanisms, directly improving the mechanical and physical properties of deposits.[1] By fine-tuning parameters like pulse amplitude and duration, a wide range of deposit characteristics - such as composition, thickness, grain size, porosity, and homogeneity - can be precisely controlled and enhanced.

This study focuses on exploring the relationship between deposition parameters and deposit properties through a combination of theoretical analysis and experimental validation. The goal is to achieve products with characteristics equal to or better than current standards while reducing metal thickness, a critical step toward sustainable industrial practices. In pulse electroplating, the deposition of nanostructures depends on two key processes: the nucleation rate and the growth of existing grains.[2] High nucleation rates, achieved through current density, and the inhibition of grain growth via specific molecules are vital for producing fine, compact deposits.

Pulsed currents have shown the potential to produce shinier and brighter films compared to steady currents, significantly enhancing deposition efficiency. Furthermore, bipolar currents excel in providing exceptional homogeneity across the deposition area and are less prone to edge effects. This research highlights the capabilities of pulsed current techniques in electroplating, presenting a pathway for industrial advancements.[3] Understanding how deposition parameters influence deposit properties can drive innovation and optimization, ultimately improving product quality and performance across diverse industrial applications.

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[3] E. Mariani et al., *Scientific Reports*, **2022**, *12*, 18175.

OR23

Characterizing Viscoelastic Properties and Confinement-Induced Dynamics in PVA-Chitosan Hydrogels

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Hydrogels (HGs) are porous materials with a 3D network structure, with applications in various fields such as filtration, selective absorption, and anti-biofouling. In this work we investigated sustainable hydrogels with tunable mechanical properties for applications in bacterial filtration. HGs composed of sustainable components, chitosan (CT) and polyvinyl alcohol (PVA), were synthesized using different compositions.[1] The viscoelastic properties of these HGs as a function of composition were evaluated using a novel approach based on squeeze-flow experiments, where compressive forces are applied.[2] Subsequently, the HGs were utilized to study the motility and dynamics of *Bacillus subtilis* (BS) bacteria in confinement, modulated by pore size. Analysis of mean squared displacements (MSDs) revealed a transition in bacterial behavior, shifting from the run-and-tumble dynamics observed in unconfined BS to progressively sub-diffusive motion, which is mainly influenced by the CT content, revealing the bacteriostatic action of CT.

Figure 1: On the left, a schematic representation of the compression test performed on the HG; on the right, the HG used to study BS bacterial motility.

[1] F. Soto-Bustamante et al., *Gels*, **2023**, *9*(5), 396.
[2] M. Tassieri et al., **2016**, *60*(4), 649-660.

OR24

Sustainability and optimization of an electroplating industry: from multilayer engineering to theoretical understanding of charge transfer processes

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To optimize and enhance the sustainability of an electroplating plant a review was done to underline the key points, visualizing how the is fundamental to understand theoretical aspects both of multilayer engineering and charge transfer (CT) processes from a chemical-physical perspective. For the first point, a study on intermetallic diffusion and barrier properties of different materials was performed thanks to a newly cost-effective analytical method based on X-ray spectroscopies (EDS and XRF) to determine the diffusion coefficient. The diffusion mechanism was also determined by the means of X-ray diffractometry (XRD). This study results in properly differentiating between anticorrosive and barrier layers and giving new hints on how develop multilayer materials to minimize the metal usage.[1] In parallel, theoretical studies of CT processes were conducted: in particular, molecular crystals were characterized benchmarking various levels of density functional theory (DFT) and population analyses, finding how the functional class and basis set influence dramatically the result. Molecular crystal structures were optimized at PAW/PBE(D3BJ) level and IR and Raman spectra were calculated from a frequency calculation and compared with experimental results, underling how the usage of pseudopotentials overestimate the ionicity of the system, leading to blueshifts.[2] Moreover, charge carriers in radical polycyclic aromatic hydrocarbons and peculiar spectral properties were characterized by exploiting several classes of DFT functionals, predicting the existence of the optical-active giant-response in vibrational circular dichroism caused by a chiral polaron. The knowledge acquired thanks to the theoretical studies was implemented in the made of a workflow to model electroplating processes and electroplating formulations.[3]

[1] F. Biffoli et al., *Helyion* **2024**, *10,* e32147.
[2] F. Biffoli et al., *J. Phys. Chem. C* **2024**, *128*, 14046-14055.
[3] F. Biffoli et al., *J. of Electroanalytical Chem.* **2024**, *972,* 118617.

OR25

The use of XPS photoelectron and Auger lines in the characterization of catalysts and their supports

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The use of X-ray photoelectron spectroscopy (XPS) is a well-established method for characterizing catalysts, as its limited sampling depth gives information on the surface atoms, which are crucial in heterogeneous catalysis. Trying to obtain a more precise picture of what happens during the catalytic step, the catalysts can be characterized in different phases: i) as the as-prepared catalyst, usually a powder, ii) as the dispersed on the support one, and then iii) activated and iv) spent. Since we are usually interested in the chemical speciation and in the quantification of the load of the catalyst, information that we can get by analyzing energy and area of the photoelectronic peaks, we need to enable protocol designed to minimize spurious effects such as the differential charging that might introduce artefacts in the line shape and to find the more suitable curves avoiding overfitting.[1] This central task requires smart sample preparation as those I will briefly report.[2] Then I will focus on the analysis of a bismuth-based and a copper-zinc oxide catalyst supported on alumina, both presenting peculiar problematics for the analysis and requiring a methodology capable of enabling their characterization. In the case of copper-based catalysts, we utilized Auger peaks to resolve the ambiguity in the Cu 2p peak position and to identify the oxidation state and chemical environments of Cu^0 and Cu^+.[3] Furthermore, these methods were adapted to address the compositional analysis of sputtered thin films and substrates decorated with metallic mono- and poly-metallic deposits. Steps necessary to follow a scheduled pathway for the assessment of the right element's oxidation state, required to outline the behavior of substrates and catalysts through the catalytic step. This work lays the foundation for future studies combining XPS with temperature-programmed desorption. The activities were partially conducted within the framework of the RESOLCAT P2022J5NAN_003 project.

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[2] ASTM, *E1523-15*, **2015**.
[3] G. Moretti et al., *Surf. Interface Anal.* **2006**, 224–228.

OR26

Innovative Smart Materials: From Reversible Shape Control to Passive Sweat Collection in Microfluidic Sensors

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Liquid Crystalline Networks (LCNs) are remarkable materials composed of mesogenic molecules chemically crosslinked into polymeric networks, enabling reversible shape changes in response to external stimuli such as light, heat, and mechanical stress.[1] These unique properties make LCNs ideal candidates for applications in actuators, sensors, and other responsive devices. In this work, the focus was on developing LCN-based actuators by tailoring the molecular composition of the liquid crystal crosslinker to achieve higher actuation intensities. Optimizing these crosslinkers led to enhanced deformation capabilities, expanding the potential applications of LCN actuators.

During the second phase of the research, the study extended to the integration of LCNs with magnetostrictive FeGa thin films, which convert mechanical stress into magnetic changes, and vice versa. Photoresponsive azobenzene-doped LCN films, capable of reversible deformation under UV and visible light, were used to transfer mechanical stress to the FeGa layer. This integration enabled precise, light-driven control of the FeGa film's magnetic properties, facilitating compact, contactless systems without the need for bulky magnets or energy-intensive coils. Further research is ongoing to explore the application of this technology in sensor development.[2]

Furthermore, my work also focused on passive sweat collection for wearable microfluidic sensors, studying different approaches to overcome the hydrophobicity of the PDMS used to allocate the sensor making it wearable.[3] The investigation regarded hydrophilic treatments, including PDMS copolymerization with PEGDA or HEMA and surface treatments with PVA or HEMA solutions, demonstrating an effective passive sweat collection.

This research advances responsive composite materials and wearable sensing technologies, with potential applications in robotics, healthcare, and environmental monitoring.

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[2] G. Barrera et al., *Adv. Sci.* **2024**, 2408273.
[3] I. A. Vitale et al., *TrAC*. **2024**, *180*, 117965.

OR27

Ferritin-based anticancers

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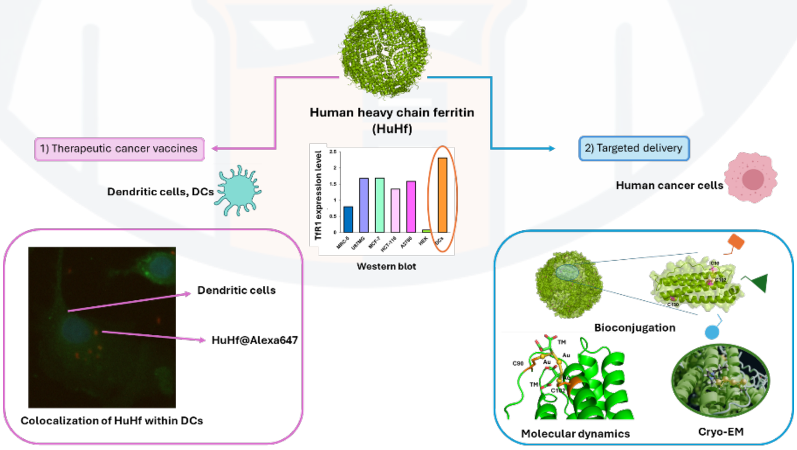
This Thesis work aimed to solve two biological problems exploiting human ferritin (HuHf hereafter) as biological tool: i) therapeutic anticancer vaccines development; ii) selective delivery of metal-based drug against cancer cells.
Regarding the first part we obtained preliminary data to demonstrate the TfR1-mediated internalization of HuHf by human dendritic cells, a proof-of-concept that poses ground bases for the development of this research work. On the second aspect, we obtained a large set of data that allowed us to develop a reproducible method to produce efficient bioconjugates between HuHf and three gold(I)-metal based drugs, i.e. auranofin,[1] aurothiomalate[2] and a monocarbene. The samples were tested *in vitro* against A2780 ovarian cancer cells gaining a deep description of their cytotoxicity and induced metabolic effects; cytotoxic information was also obtained on other human cancer cell lines. With the use of a variety of biophysical techniques we obtained structural information that led us to the identification of the binding sites of the three different gold(I) compounds, which resulted in peculiar mode of binding.



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[2] L. Cosottini *et al.*, *Angew. Chem. Int. Ed.*, **2014**, 410791.

OR28

Oxygen Reduction Reaction Catalysts from Electroplating Industries Waste Solution

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[b] Department of Human Sciences for the Promotion of Quality of Life, University San Raffaele Roma, Via di Val Cannuta 247, 00166-Rome, Italy
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The progressive depletion of fossil reserves and the increase in energy demand have led to a rise in fuel and electricity prices. In this context, fuel cells are promising candidates for a sustainable future. Oxygen Reduction Reaction (ORR) is the bottle-neck strategic reaction ruling the fuel cell efficiency process. However, the slow kinetics of ORR require highly effective electrocatalysts for proper boosting [1]. This study focuses on obtaining low-content platinum-group metals catalysts recovering precious metals from electroplating industry wastewater using carbon black and graphene substrates functionalized with the pyrimidine TREN derivative. The functionalization significantly increased both the Pd recovery and the catalytic properties. The results of the rotating ring-disk electrode (RRDE) experiments confirmed a four-electron pathway, with no significant formation of hydrogen peroxide during the ORR. In addition, a Pd(II) complex of a tetraazacycloalkane anchored to multi-walled carbon nanotubes was tested in order to verify whether Pd(II) must have free coordination sites to function effectively in ORR reactions or whether, as predicted by the theoretical work [2], the catalytic effect may result from an O_2 interaction at the fifth coordination position. The tetraazacycloalkane ligand was chosen to saturate the four coordination sites of the typical square planar coordination geometry of Pd(II), obtaining that the tetracoordination of Pd(II) does not influence its catalytic capacity and enhance the robustness of the catalyst. The onset potential value and the half-wave potential of the catalyst are, respectively, only 53 mV and 24 mV less positive than those observed for a Pt electrode and the direct conversion of O_2 to H_2O reaches 85.0% showing that these approaches promote the development of a circular economy and provide a basis for further development to improve the efficiency of future low-cost catalysts for alkaline fuel cells.

[1] Y. Li et al., *Energ. Rev.* **2019**, *2*, 518-538.
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OR29

Biomimetic Nanoarchitectures for Aerosol Treatment

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The aim of the research is the development, the preparation and the characterization of biomimetic nanoarchitectures for aerosol-based treatment of cancer as well as coronavirus-related diseases. The study employs three different receptors selected to bind key proteins involved in these pathologies and their encapsulation into liposomes for direct delivery to the lungs (**Figure 1**).

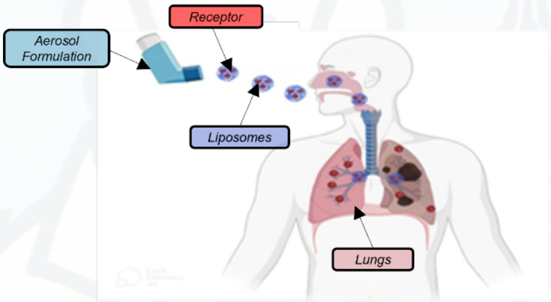

Figure 1: Schematic representation of the project.

Specifically, we evaluated the efficacy of ELTEN378 and FK506, respectively a synthetic and a commercially available receptor for the FKBP12, a protein implicated in cancer genesis.[1] Additionally, we designed and synthesized ASH79 a receptor able to selectively binds NSP13 protein,[2] that, in turn, plays a key-role in virus activity of all coronaviruses. We developed biomimetic systems and studied the drug inclusion via Langmuir monolayers and Brewster Angle Microscopy at the air-water interface, and fluorescence spectroscopy on Langmuir-Blodgett films. Furthermore, we prepared and characterized liposomes composed of DPPC/POPG 8:2 to encapsulate the receptors, enabling delivery directly to the lungs for therapeutic applications.

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[2] P. Procacci et al., *ChemMedChem*, **2014**, *19*.

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OR30

Development of peptide nucleic acids-based molecules targeting G-quadruplex structures

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G-quadruplexes (G4) are non-canonical nucleic acids structures predominantly found in guanine-rich sequences and notably present in the promoter regions of oncogenes and telomeres, making them relevant targets in cancer therapy.[1] The stabilization of telomeric G-quadruplexes, for instance, can inhibit telomerase activity, inhibiting telomere elongation and ultimately leading to cancer cell death. In this context, numerous ligands have been developed to stabilize G4 structures, disrupting related biological pathways, though many still lack sufficient selectivity.[2] Recently, peptide nucleic acids (PNAs), which feature natural nucleobases attached to a polyamide backbone, have gained attention for their potential in targeting nucleic acids. Their structure allows for stable binding to nucleic acids and resistance within biological systems.[3] The ultimate objective of this project is the design PNA-based molecules to selectively target DNA G-quadruplexes to stabilize their configuration. In particular, the fundamental concept driving this project is to synergize the base-pairing selectivity of PNA molecules with the capability of G4-ligands to stabilize G4s. In the work conducted so far, the synthesis of four PNAs, each based on a telomeric DNA sequence, has been optimized with the goal of forming heteroquadruplex structures through interaction with telomeric DNA. Additionally, a PNA designed to form a PNA-DNA complex, incorporating both a PNA-DNA heteroduplex and a PNA-DNA heteroquadruplex, has also been successfully synthesized. We report the PNAs synthesis and the circular dichroism studies to define the topology of PNA-DNA heteroquadruplexes, the stoichiometry of the obtained DNA-PNA complexes, and the melting temperatures of the resulting complexes. We also report in silico studies aimed at evaluating the key interactions driving the formation of heteroquadruplexes. These analyses were conducted to identify potential modifications in PNA structures that could enhance their stability within DNA-PNA complexes, and to guide the subsequent design of optimized ligand-PNA conjugates.

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OR31

Precision cancer therapy: strategies to selectively inhibit the biosynthesis of cancer associated glycans

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Changes in the glycosylation patterns of the glycocalyx are orchestrated by the aberrant activity of glycotransferases (GTs) and are recognized as a cue of cancer pathogenesis.[1] These alterations are non-random and result in the creation of key cancer-associated glycan determinants that act as active drivers in malignant processes. Cancer-associated glycans help tumors to grow, spread and evade the immune system, therefore approaches that affect their biosynthesis may have a major impact on precision cancer treatment paving the way for a new road for cancer drug discovery. In this context, sialyl- and fucosyltransferases (STs and FTs, respectively) are GTs implicated in the creation of some of these cancer-associated glycans such as the Lewis's antigens.[2]

In this communication, we describe an efficient chemical approach that can allow easy access to a family of glycomimetic compounds that will be investigated as inhibitors of STs and FTs.[3] The presence of different isoenzymes within STs and FTs family highlights the need for a precision inhibition of the key STs/FTs involved in the creation of the specific Lewis antigens. Accordingly, the availability of a versatile synthetic strategy that can ensure structural variability in the glycomimetic compounds can allow to explore the space around the catalytic sites of the enzymes and to reach the ambitious goal of the selective inhibition of the target STs/FTs isoenzymes.

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OR32

Exploring Glycopeptide and Glycoprotein Structure and Dynamics. A Computational Study: from Classical Methods to Machine Learning Approaches

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This project focuses on computational glycobiology, emphasizing the structural and dynamic analysis of glycopeptides. Central to the research was the development of a novel force field for biosolvents (HFA, HFIP, TFE) to more accurately simulate peptide behavior in environments that stabilize secondary structures.[1]

A significant component of the study involved a comprehensive Python-based analysis of the Protein Data Bank (PDB), identifying over 80,000 glycoprotein structures. These were clustered using UMAP[2] and HDBSCAN based on geometrical invariant descriptors, offering an in-depth view of structural variability. Benchmarking density functional theory (DFT) methods informed the reparameterization of force fields, specifically for glycan moieties, thereby enhancing the modeling accuracy of immunologically significant peptides.

The research extended to studying the TCR-pMHC complex, with a particular focus on multiple sclerosis-related antigens such as MOG and NFL. By integrating machine learning, DFT, and bioinformatics, the study provided a novel approach to analyzing glycopeptide conformations.

Looking forward, the project aims to establish an online database cataloging glycopeptide secondary structure variations and to develop a specialized force field for glycan simulations. These efforts will supply essential tools to advance understanding of the structure and function of glycopeptides and glycoproteins.

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OR33

Dual-Targeting Anticancer Agents: Design and Evaluation of Compounds Targeting Carbonic Anhydrase and Histone Deacetylase

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The onset and progression of tumor growth involve numerous aberrant proteins and signaling pathways, highlighting the complexity of developing effective therapies. While traditional single-target drugs are often used in combination, designing chemical entities with multifunctional pharmacological properties offers distinct advantages, including enhanced patient compliance and more predictable pharmacokinetics.[1] Here we report a series of compounds designed to merge within a single chemical scaffold the prototypic inhibitor moiety of Carbonic Anhydrase (CA) (i.e. the primary sulfonamide) and Histone Deacetylase (HDAC) (i.e. the benzamide).

CAs are a family of metalloenzyme that catalyze the reversible hydration of carbon dioxide to bicarbonate ions and protons. Among the human (h) CAs, the membrane-bound isoforms IX and XII are recognized as significant solid tumor markers being overexpressed in various cancer cell lines.[2]

On the other hand, HDACs are a class of enzymes that regulate the expression of genes involved in tumorigenesis by removing acetyl groups from histones, leading to chromatin conformations that repress tumor-suppressor gene transcription.[3]

The synthesized compounds were evaluated for their ability to inhibit the most clinically relevant human CA isoforms. Additionally, their binding modes in complex with hCAs II (the most abundant physiological isoform) and XII-mimics were elucidated using X-ray crystallography. These findings contribute to the rational design of dual-targeting anticancer agents and highlight their potential as innovative therapeutic strategies in oncology.

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OR34

Repurposed and novel molecules in photodynamic therapy with antimicrobial activity

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Photodynamic therapy (PDT) involves the use of photosensitizer molecules that irradiated with low-power lasers can release radicals that, reacting with oxygen, can kill microorganisms. The main targets of PDT are the external microbial structures, namely the cell wall, cell membrane, capsid, and virus envelope. The great potential of this therapeutic approach to treat bacteria, fungi, viruses, and parasites has increased the number of scientific studies aimed at expanding knowledge in this regard.[1] The goal of our research is both to use photosensitizer molecules already in clinical use and to synthesize new classes of compounds to treat diseases for which current treatments are inefficient or otherwise have various side effects. Rose Bengal, a photoactive molecule already in use for the diagnosis of some ophthalmic diseases, was the starting point.[2] This compound was covalently and noncovalently bonded to nanocellulose, a novel nanometer-sized material that can be extracted from waste sources and/or produced by some bacteria, to realize delivery systems to transport Rose Bengal into nails for the potential treatment of onychomycosis. Our efforts have also been directed toward obtaining new water-soluble photosensitizer compounds with good cell permeability. Taking advantage of the research group's experience in the synthesis of BODIPY core products, organic dyes with interesting optical properties, innovative molecules were synthesized with this scaffold to improve some useful properties for their use as antimicrobial agents.

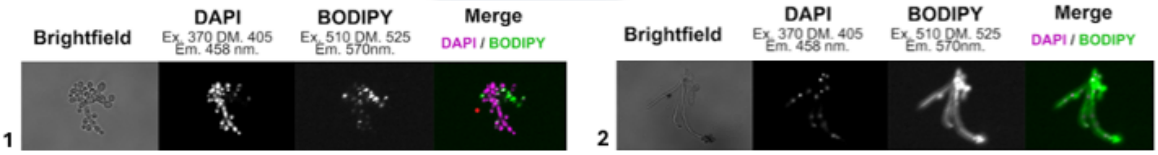

Figure 1: Internalization in C. Albicans of two novel BODIPY scaffolds compounds (**image 1**, **image 2**) using DAPI as a contrast fluorophore

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OR35

Wound Management: the importance of prevention and of appropriate treatments

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Wounds are defined as damage to the integrity of one or more body tissues and are classified as acute or chronic based on their healing time. Acute wounds heal within 8-10 weeks, after this period, they are defined as chronic. Wound management involves a comprehensive approach to the prevention, assessment, and treatment of wounds.

The prevention phase focuses on strategies to prevent wounds and ensure effective healing through proper care and monitoring; the need to prevent ulcer formation is a key factor. The other key factor in wound management is to enhance the healing process through the correct management of wound bed, the exudate and the microbial activity.

This project aims to evaluate wound dressings based on wound management needs, starting with current standards (EN 13726) and designing new test methods, like pressure mapping test. This test helps to verify how dressings can act in terms of pressure ulcer prevention and identify the best options.

Regarding the treatment of chronic wounds, as primary wound dressings, a solution could be to use a paste, that is a thick formulation with a semi-solid consistence, recommended for heavy exuding wounds; or a hydrogel, a network of hydrophilic polymer chains that contain up to 90% water, ideal for dry or low exuding wounds. A particular type of paste, Askina® Calgitrol® Paste, consisting of an ionic silver alginate matrix, is manufactured at B.Braun site in Mirandola (MO). It is a class III medical device. When applied to a wound, it interacts with wound exudate, to form a gel-like substance, that maintains a moist environment and absorbs excess exudate. As all the other advanced medications, also Askina® Calgitrol® Paste is under EN 13726:2023 standard.[1-3]

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OR36

New strategies for the monitoring and the inhibition of metals and alloys corrosion in Cultural Heritage

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In humid and polluted environments, outdoor artistic bronze preservation can be compromised by corrosive processes. Among the most aggressive forms of degradation is "bronze disease", a cyclic and autocatalytic process, resulting in surface pitting and, in severe cases, material loss. Bronze disease has been addressed from two key perspectives: first, through the application of a multi-analytical approach for the early detection of corrosion, using non-invasive and portable/transportable techniques; and second, by developing new "greener" materials, such as coatings and corrosion inhibitors.

Artificial corrosion products were characterized by employing Fiber Optics Reflectance Spectroscopy, Spectral Domain Optical Coherence Tomography (SD-OCT), laser-scanning profilometry, multispectral scanning reflectography, active IR thermography, and Electrochemical Impedance Spectroscopy (EIS). Confocal Raman Microscopy (CRM) and Scanning Electron Microscopy (SEM) allowed data validation. The combined application of these techniques provides an in-depth characterization of patinas, and promising data for the early detection and monitoring of bronze corrosion [1].

A library of new PS-MA polymers was synthesized from waste polystyrene (PS) via acylation with maleic anhydride (MA), resulting in carboxylic pendants [2]. The MA feed variation modulated polymer properties and architectures. PS-MA showed improved adhesivity, corrosion protection, and solubility in green solvents compared to pristine PS and commercial acrylic polymers. A preliminary study explored further modifications of PS-MA with oxime moieties. Finally, a new inhibitor, the 1,3,5-benzene-tricarbaldehyde trioxime was synthesized and tested. Materials were characterized using Nuclear Magnetic Resonance, Attenuated Total Reflection Fourier Transform Infrared Spectroscopy (ATR-FTIR), Differential Scanning Calorimetry, Thermogravimetric analysis, Size Exclusion Chromatography, and performing solubility tests. EIS, SD-OCT, colorimetry, ATR-FTIR spectroscopy, and CRM characterized applicative performance.

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OR37

Exploring the potential of metal-based compounds against multidrug resistant pathogens: the case of *Burkholderia cenocepacia*

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Bacteria belonging to the *Burkholderia cepacia* complex (Bcc) are notorious Gram-negative opportunistic pathogens, particularly problematic for individuals with cystic fibrosis[1]. These bacteria, like *Burkholderia cenocepacia*, possess elaborate evasion mechanisms against multiple classes of antimicrobials, which are also responsible for the significance of their infections. For these reasons there is an urgent need for novel antibiotics that can counter the escalating threat posed by antibiotic-resistant bacteria. One strategy to tackle this crisis involves repurposing existing drugs, such as gold(I)-based drug, which are known to possess high affinity towards proteins' free thiols and have shown bactericidal activity against Gram-positive bacteria, like auranofin.[2] Auranofin achieves this by inhibiting thioredoxin reductase (TrxB) and disrupting the cell's ability to endure oxidative stress. However, its effectiveness is limited against many Gram-negative bacteria, with the reasons not entirely clear—whether it's due to variances in cell envelope permeability or the presence of glutathione reductase (GOR), an enzyme which is functionally and structurally similar to TrxB.

Here we investigate the effects of the treatment with a selected panel of commercial and novel synthesis gold- and silver-based compounds on two patient-isolated strains of *B. cenocepacia*. We also evaluate the reactivity of some of these metal-based compounds towards the main intracellular target, which is thioredoxin reductase, through an ESI-MS approach. The protein was obtained via heterologous expression in *E. coli* cells. Generally, the analysis of the obtained spectra revealed the formation of stable adducts. Overall, the present results set the stage to better understand the mechanism of action of these compounds and to elucidate their antimicrobial activity.

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OR38

Peptide Inhibitors of SARS-CoV-2 Cell-Entry: Synthesis, Structural Analysis, and Biological Evaluation

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Despite the availability of vaccines, COVID-19 remains aggressive, particularly in immunocompromised individuals. Hence, the imperative for developing a specific therapeutic agent with antiviral activity against SARS-CoV-2 persists. The entry mechanism of SARS-CoV-2 into cells is intricate, relying on molecular events susceptible to targeting for blocking cell infection. The viral spike glycoprotein, situated on the surface of the viral membrane envelope, is a pivotal player in this process. The infection cascade commences with the receptor binding domain (RBD) of the viral spike protein engaging with the angiotensin converting enzyme 2 (ACE2), which serves as a host receptor for the RBD expressed on the host cell surface. Notably, the crucial residues for this interaction are located in the helix α1, specifically ACE2(24-42). To stabilise this important secondary structure, we synthesized several triazolyl-bridged ACE2(24-42) analogs exploiting copper(I)-catalyzed azide–alkyne cycloaddition (CuAAC).[1] Among these stapled peptides, the one bearing the triazole-containing bridge at positions 36–40 exhibited promising antiviral activity at micromolar concentrations, as evaluated by plaque reduction assay (PRA). Conversely, the double-stapled analog demonstrated a loss of activity, suggesting that excessive rigidity hinders interaction with the RBD.[2] Another critical step in SARS-CoV-2 cell entry is membrane fusion, wherein the interaction between the Internal Fusion Peptide (IFP) and the Membrane Proximity External Region (MPER) in the S2 subunit of Spike plays a crucial role. The peptide Spike(888-906), encompassed within the IFP sequence, displayed significant antiviral activity in vitro (IC50: 0.20 ± 1.11 μM). Surface Plasmon Resonance (SPR) revealed a high affinity of this peptide for the MPER fragment (Kd= 9.44 nM). Finally, Ala-scan analysis underscored the key role of aromatic residues in the antiviral activity.[3]

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OR39

Non-lamellar Lipid Nanoparticles as Innovative Vectors for RNA Delivery

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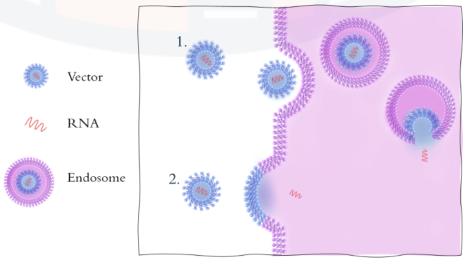
Gene therapy and RNA-based drugs is a strategic research area for the development of innovative therapies. To promote its application, RNA's inherent limitations must be overcome by designing delivery vectors to protect the RNA cargo from the environment and precisely release it to its biological target.[1] Among such systems, lipid nanoparticles (LNPs) are particularly promising. To boost their clinical translation, careful design of the LNP composition and structure is key to ensure: (i) an efficient complexation of RNA and (ii) the ability of LNP-RNA complexes to cross the plasma membrane, escape from the endosomes and release the RNA[2,3] (Figure 1). To this aim, attaining a deep physicochemical understanding of these systems is crucial, as well as investigating their behavior towards biological interfaces. In this contribution, new formulations of non-lamellar LNPs-based vectors are presented. The cationic nature of the LNPs is designed to efficiently bind RNA and the topological characteristics of these LNPs (cubic or hexagonal geometry) are designed to enhance the endosomal escape of the lipoplexes. To test their potential as RNA carriers, their structural, colloidal, and functional properties were characterized using DLS, ζ-Potential, SAXS and QCM-D. Furthermore, very promising results were obtained from transfection studies on HEK 293 cell line. The results presented will contribute to improving the understanding of the physicochemical properties of LNPs vectors and their interaction with biological membranes, promoting their potential application as therapeutics.



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OR40

Development and Optimization of Self-Assembling Modified Beta-Cyclodextrin-Based Nanocarriers for gene delivery

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The advancement of gene delivery systems is crucial for optimizing RNA-based therapies. This study presents a novel approach utilizing self-assembling modified beta-cyclodextrin (β-CD) nanocarriers specifically designed for siRNA transport. Collaborative efforts between the University of Florence and the University of Santiago de Compostela led to the exploration of three distinct cationic β-CDs (designed and synthesized by CharboHyde Zrt., Budapest, Ungary), each featuring primary amino groups on the secondary rims and varying lipophilic chains on the primary side.

Comprehensive characterization of these β-CDs was performed using X-ray diffraction, differential scanning calorimetry, infrared spectroscopy, and Nuclear Magnetic Resonance, confirming their structural integrity. Solubilization studies identified optimal conditions for nanoparticle (NP) formation, followed by assessments of complexation efficiencies with plasmid DNA and siRNA. Characterization of the resulting NPs indicated that CD1 and CD2 exhibited favorable properties for gene delivery, maintaining desirable size and polydispersity index.

Stability assessments demonstrated that the NPs remained stable over time, while transmission electron microscopy provided visual confirmation of their morphology. Cytotoxicity assays confirmed the biocompatibility of the β-CD nanocarriers across various cell lines, including pancreatic MIN-6 and HeLa cells. Additionally, the transfection capacity of the nanoparticles was evaluated on HeLa cells, confirming the potential of this formulation.[1-3]

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[2] R. M. Haley et al., *Drug Deliv. Transl. Res.* **2020**, *10*, 661-677.
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OR41

Synthesis of innovative nanomaterials to develop improved Rare Earths-free permanent magnets

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Moving towards greener and more sustainable technologies, nowadays the development of permanent magnets (PMs) not based on rare earth elements (REEs) is constantly on demand. PMs constituted by rare earths stand out for their considerable performances expressed, but the high cost, the supply risk, and environmental issues associated with their production lead to the research of new materials and improvements in the functional properties of the existing ones. The global market of PMs is mainly split by NdFeB and hexagonal ferrites, but ferrite hard magnets, especially Sr-hexaferrite (SrM), present several economical and technical advantages that can make them eligible to be an alternative to REEs-based magnets, despite in comparison they are quite low in performance.[1] They exhibit, indeed, relatively large coercivity (H_C), but modest saturation magnetization (M_S), and remanence (M_R).[2] Consequently, the improvement of these SrM properties can fil, at least partially, the huge gap that separates them from REEs, giving a more sustainable option for future engineering.[3] The work here presented moves in this framework aiming to enhance the properties of SrM by synthesizing and obtaining aligned nano-sized grains and developing valuable and sustainable strategies for the industrial production of high energy product ferrite PMs not relying on REEs content. The investigated approaches comprise different paths: the control of the nanoparticle size (below 100 nm) tailoring the synthesis route (solid-state, sol-gel) and the relative process parameters; modify the magnetic or morphological features of SrM by doping with suitable elements (i.e. Al, Mn); the incorporation of a different synthesized material as Fe° nanowires to enhance the magnetization value through exchange-coupling effect, and innovative densification techniques like spark plasma sintering (SPS) to prevent the grain enlargement. Moreover, the industrial manufacturing processes involved in the bonded magnet production during the abroad experience in Slovenia will be also shown.

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OR42

Development and characterization of emulsion-templated PDMS organogels for modern and contemporary artworks cleaning

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Traditional conservation methods to remove unwanted surface layers from modern and contemporary artworks often involve mechanical or solvent-based cleaning, which can damage the artwork, mainly due to lack of selectivity, and posing environmental risks. The aim of the project is to set up a new family of chemical organogels and sponges with customizable mechanical properties and porosity to remove unwanted surface layers from modern and contemporary artworks. By confining solvents within the micro- and nano-porosity of viscous gels, selectivity and control improve, helping to protect the original materials.

Emulsion templated macroporous xerogels based on Polydimethylsiloxane (PDMS) are synthesized by polymerizing the continuous phase of a w/o microemulsion, using the created droplets as templating agents to generate the porosity.[1] The aqueous dispersed phase is made by a solution of $NaHCO_3$, that undergoes a thermal decomposition, with the formation of CO_2. Then, during the curing process of the PDMS matrix (carried out at 60°C), the produced CO_2 creates a specific porosity into the 3D polymeric network. Different amount of microemulsion were added into the PDMS pre-polymer mixture, and the final formulations were characterized by FTIR-ATR to evaluate the chemical structures, and to verify the absence of surfactant after the synthesis. The structural and morphological characterization of the obtained systems was carried out by means of Scanning Electron Microscopy (SEM) and X-tomography, while the water-in-oil microemulsions were characterized by means of DLS to evaluate the dimensions and the size distribution of the nanodroplets.

To evaluate the capability of the PDMS based gels to adsorb and retain organic solvents and to assess possible correlations with solvent polarity and internal porosity, both swelling and release studies were carried out. Then the experimental data were fitted using different models.[2]

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OR43

Computational Exploration of Magnetic Exchange in Transition Metal Molecular Spin Qubits: From Isolated Molecules to Bulk Phases

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Transition metal coordination complexes of Copper(II) and Vanadyl(IV) are promising candidates for molecular spin qubits, owing to their tunable synthesis and long coherence times.[1] These features make them highly attractive for quantum computing applications. To advance quantum technologies such as computing, sensing, and communication, it is crucial to address challenges such as decoherence, the development of multi-qubit architectures, and the precise control of magnetic exchange interactions (***J***). The latter is particularly crucial, as the exchange interactions between qubits are not only the natural resource of the entanglement, but they can solve the qubit's connectivity when superexchange is considered. Indeed, if double qubits can give a universal gate set for quantum computation (along with single ones), higher connectivity is also advantageous for quantum error correction. In this perspective, we examine magnetic superexchange interactions by ab initio approaches in selected systems, both in their bulk and gas phases. For the bulk phase, we focus on two systems: (i) a sulfur-rich antiferromagnetic [Cu(dttt)$_2$] complex [(dttt)$^-$ = 1,3,2-dithiazole-4-thione-5-thiolate),[2] and (ii) a V^{IV}O-Cu^{II} porphyrin-based [VOCu(DPP)$_2$] complex [(DPP$^-$ = diphenyl porphyrinate)] with weak ferromagnetic interaction.[3] By incorporating periodic boundary conditions, we evidenced the role of packing interactions with the earlier gas-phase DFT calculations. Accurate ***J***-values are achieved by applying Hubbard correction (DFT + U) computed through Linear Response Theory. For the isolated phase systems, our focus will be on TrPP-based Vanadyl Porphyrins appended to photoexcited organic chromophores, specifically the meso-meso linked dimer of Vanadyl Porphyrin and free-base porphyrin [VO-FP]. We aim to explore and compute the specific magnetic interactions involved in the spin dynamics of their photophysical pathways. Additionally, in the DPP analogue of the VO-FP system, we investigate the electronic and optical properties, as well as the magneto-optical Kerr effect, conducted as part of the abroad mobility study.

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OR44

Sustainable Nanostructured Coatings for the Conservation of Street-Art

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Street-art conservation faces the challenge of balancing the need to protect artworks from environmental degradation while preserving their aesthetic and structural integrity.[1] This study examines the development and evaluation of a hybrid protective coating that combines chitosan, a sustainable, biodegradable biopolymer,[2] with nanosilica, an inorganic material recognized for its mechanical strength and stability. This hybrid formulation is designed to meet the specific requirements of Street-art conservation, such as compatibility with various substrates, resistance to UV light, temperature and humidity, and preservation of surface breathability. Chitosan was dissolved in an acidic solution to synthesize the coating, the pH was almost neutralized, and silica nanoparticles were added. Concrete mock-ups that mimic Street art substrates were spray-painted with acrylic and alkyd paints and then coated with the hybrid formulation. To assess its performance, the samples underwent extensive characterization and accelerated aging tests that simulated environmental stressors, including UV exposure, high humidity, and temperature. Fourier Transform Infrared Spectroscopy (FTIR) confirmed the chemical stability of the coating while Scanning Electron Microscopy (SEM) revealed smooth, defect-free film morphology. Dynamic Light Scattering (DLS) and zeta potential analyses confirmed the hybrid solution's stability during application. Performance tests showed minimal color changes, improved adhesion as determined by tape tests, and unchanged water vapor permeability, indicating that the coating can protect while maintaining substrate breathability. The hybrid coating would be further evaluated through real-world applications, including the monitoring of SKIM's "Anna Maria" mural, a 290 m^2 street art piece located in Sesto Fiorentino, 2023, Italy. Observed degradation patterns, such as color fading, efflorescence, and cracking, highlighted the need for durable protective strategies. The hybrid coating showed promise in addressing these issues, supported by artificial aging experiments conducted on mock-ups that replicated the mural's materials and techniques. Additionally, the chemical characterization of the spray paints employed by the artist is presented.

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OR45

Electrochemical Strategies and Electrodeposition Techniques for Advancing Decorative Electroplating Applications

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This PhD research explores innovative electroplating methodologies for decorative applications, aiming to enhance economic and environmental sustainability. The study encompasses two primary objectives: (1) the development of an electrochemical method for quantifying organic additives in acid copper electroplating baths and (2) the identification of key parameters influencing hydrogen incorporation and retention during palladium electrodeposition. In the first research area, an Electrochemical Impedance Spectroscopy (EIS) method, combined with Distribution of Relaxation Times (DRT) analysis, was developed to address limitations of traditional additive quantification techniques such as ion chromatography and the Hull cell. The new methodology, based on a single EIS measurement, utilizes DRT to extract time constants correlated with additive concentrations, analyzed via statistical modeling. Results demonstrated high accuracy and reproducibility,[1] offering a more sustainable and efficient approach. Additionally, a novel spectrophotometric method for chloride ion quantification in acid copper baths was validated, surpassing existing titration techniques in precision and efficiency.

The second research focus examines hydrogen incorporation during palladium electrodeposition, a critical factor influencing the structural integrity of deposits. Palladium's ability to absorb hydrogen forms two hydride phases: α-PdH_x and β-PdH_x differentiated by hydrogen content and lattice size. The β -phase, prone to gradual hydrogen desorption, induces lattice contraction, risking deposit fracturing.[2] Systematic X-ray diffraction (XRD) analyses of samples with varying thicknesses and current densities were conducted at intervals post-deposition to evaluate desorption kinetics. Results facilitated the creation of operational maps for phase-selective deposition. Pulsed and reverse-pulsed deposition techniques were also explored, yielding distinct outcomes compared to direct current methods.

This work aims to provide practical insights and innovative tools for the electroplating industry. It advances the understanding of hydrogen incorporation mechanisms and proposes sustainable alternatives for additive quantification. These contributions not only enhance process efficiency but also align with broader environmental and economic objectives in decorative electroplating. Further research will refine these methodologies and explore their scalability for industrial applications.

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OR46

Enhancing the rotating magnetocaloric effect in lanthanide complexes via high order magnetic anisotropies

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Lanthanide-based metal complexes exhibit unique properties that make them highly suitable for applications in fields such as information technology and material sciences. One critical property is magnetic anisotropy, *i.e.* the directional dependence of their magnetic response. A notable application leveraging on this property is the Rotating Magnetocaloric Effect (RMCE), a phenomenon enabling efficient cooling by rotating an anisotropic material in a fixed magnetic field. This rotation increases the magnetic entropy of the system, producing a decrease of the temperature of the environment, allowing to perform a cooling cycle.[1] Typically, RMCE utilizes easy-axis anisotropy which requires a 180° rotation to complete a full cycle. In contrast, high-order magnetic anisotropies, such as tetragonal or hexagonal, can complete a cycle with smaller rotations (90° or 60° respectively), offering potential enhanced efficiency.

To explore this possibility, we synthesized three novel *3d-4f* metal complexes based on the DOTA archetype.[2] The general formula of the complexes is *trans*-$[MF_2(py)_4][LnDOTA]$ ($M = Cr^{3+}$ or Co^{3+}, $Ln = Dy^{3+}$ or Y^{3+}, py = pyridine and DOTA = tetraazacyclododecane-N,N′,N′′,N′′′-tetraacetate). A combination of single-crystal DC magnetometry, torque magnetometry and DFT calculations confirmed the tetragonal magnetic anisotropy of the *4f* unit. Angular-resolved magnetometry of an ordered ensemble of single crystals provided proof-of-concept data, demonstrating the feasibility of our approach. These findings highlight a promising strategy for developing the next-generation magnetic coolants.[3]

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[3] L. Tacconi et al., *Angew. Chem. Int. Ed.*, **2024**, e202417582.

OR47

Ultra-low temperature magnetic investigation of a single molecule magnet on a type-II superconductor

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Magnetic molecules offer a versatile playground for exploring quantum effects in magnetism at the nanoscale. Recent research has focused on depositing intact magnetic molecules on surfaces while preserving their functional properties, paving the way for their integration into solid state devices for future quantum technological applications.[1] The aim of my PhD is to investigate the structural, electronic and magnetic properties of hybrid molecular systems deposited on conductive and superconducting surfaces through a multidisciplinary approach, including in-house techniques (STM, AFM and XPS) and X-ray absorption spectroscopy at large-scale facilities. The combination of superconductors (SCs) with magnetic materials, including magnetic molecules, revealed the appearance of novel physical phenomena, and low temperatures are of primary importance in investigating them.[2] During the first year of my PhD, we exploited the ^{3}He-^{4}He dilution refrigerator available at the DEIMOS beamline (SOLEIL synchrotron) to investigate the behaviour of an iron-based single molecule magnet (SMM) deposited on a type-II SC, the $NbSe_2$ substrate. The dichroic measurements with soft X-rays at sub-kelvin temperatures confirmed that SMMs retain their hysteretic behaviour on the surface and show the signature of the Meissner screening of the substrate. This effect, previously observed for lead, is ascribed to the switching of the SMM layer from a blocked magnetization state to a resonant quantum tunneling regime occurring at the superconducting transition.[3] These measurements show the enhanced sensitivity of SMMs to SC transitions occurring even at very low magnetic fields, such as the H_{C1} of type-II SCs.

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OR48

Multiresponsive Ionic Conductive Alginate/Gelatin Organohydrogels with Tunable Functions

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The immense application potential of wearable electronics has triggered an increased research effort on the development of new multifunctional materials combining stretchability and sensitivity to external stimuli. Among flexible and stretchable materials, conductive hydrogels have gained a great research interest during the last decade.[1] The use of ionic conductivity for sensing is recently emerging as powerful strategy enabling the use of polymeric matrices that are not intrinsically conductive, without the addition of carbon-based fillers that affect the transparency of the final products. This approach enables the design of stretchable sensors based on biopolymeric compounds. Biopolymers offer in fact interesting opportunities for the development of responsive wearable devices, since they are cheap and particularly sensitive to the surrounding environment. Among the biopolymers, gelatin and alginate can be used for this purpose if properly processed: gelatin is a polypeptide capable of forming hydrogels particularly sensitive to temperature, while alginate is an exopolysaccharide that possesses high reactivity and selectivity towards metal cations with various oxidation states.[2] In order to foster the use of biopolymer-based stretchable sensors, we developed a simple and reproducible preparation for transparent ionically conductive gelatin-alginate organohydrogels responsive to multiple stimuli. Gelatin was used to provide stretchability and thermal responsivity, while alginate was crosslinked with di-, tri- and tetravalent cations (namely Mn^{2+}, Cu^{2+}, Fe^{3+}, Zr^{4+}) to modulate both the mechanical properties and the ionic conductivity of the devices. The latter proved to be responsive to temperature, humidity, strain and light. TGA, DSC, SAXS and mechanical analyses highlighted the different physico-chemical properties of the gels that result in different sensitivity to the four stimuli previously listed. The possibility to easily tune the responsivity as a function of the chosen crosslinker and the high sensitivity reached suggest promising perspectives for the use of our devices as wearable stretchable sensors.

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OR49

Valorization of Rapeseed Meal Proteins to Developing Sustainable Biodegradable Composites

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The agri-food industry generates substantial biowaste, often discarded or used as animal feed, yet rich in bioactive compounds with potential for several applications.[1] This study aims to valorize rapeseed meal biowaste, a byproduct of oilseed production, to develop biodegradable, protein-based composites with industrial applications, supporting a shift towards a circular bioeconomy. We developed a scalable, eco-friendly protein extraction process, yielding a high-quality protein-enriched extract. Through intermediate pyrolysis, the protein extraction residue was converted into bio-oil and bio-char, enabling full resource recovery aligned with circular economy principles.[2] The study introduces a method for producing flexible biomaterials from raw, protein-rich rapeseed meal, utilizing crosslinking with epoxides and compression molding. Protein blends with glycerol, cross-linker, and denaturants were thermally processed to improve material strength and durability.[3] Moreover, collagen and rapeseed meal protein hydrolysate from enzymatic proteolysis was incorporated to enhance flexibility and reduce water permeability. Mechanical and thermal properties of the composites were optimized by adjusting ratios of rapeseed meal protein and collagen hydrolysates, which acted as effective plasticizers.[3] Our findings demonstrate that rapeseed meal-based materials can be tailored to meet industrial demands for biodegradable alternatives. This work represents an initial step toward sustainable, cost-effective bio-based materials, promoting the recovery and valorization of agricultural byproducts within the framework of a circular economy.

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OR50

Recognition of emerging pollutants (EPs) with artificial fluorescence chemical sensors: a supramolecular approach

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The concept of "emerging pollutants" (EPs) refers to chemical compounds not currently included in routine environmental monitoring, but potentially posing significant risks to ecosystems and human health.[1] This doctoral project focuses on the design, synthesis, and characterization of novel fluorescent chemical sensors, with the aim to detect the most relevant classes of EPs, including pharmaceuticals, such as antibiotics and non-steroidal anti-inflammatory drugs (NSAIDs), as well as waterproofing agents, like perfluoroalkyl substances (PFAS). A range of luminescent polyamine-based chemosensors was developed utilizing a receptor-spacer-fluorophore modular approach for which the interaction between the guest molecule and the receptor unit as a result of appropriate combination of specific intermolecular interactions, may induce changes in the luminescence emission of fluorescent chemosensors.[2] In the present study we have evaluated the optical responses of these chemosensors towards selected analytes within the categories of NSAIDs, antibiotics, and PFAS, by monitoring different mechanisms such as fluorescence quenching by photoinduced electron transfer (PET) or Förster energy transfer (FRET). Of note, the probes developed throughout this project demonstrated selective detection capabilities, being able, in several cases, to recognize single analytes in complex matrices. In the course of our work on chelating moieties linked to signaling units, we also synthesized fluorescent chelating agents designed for multimodal imaging applications, combining positron emission tomography (PET) and optical fluorescence imaging (OFI). To this purpose, we developed new Zr(IV), and Cu(II) deferoxamine-based fluorescent chelating agents which demonstrated retention of fluorescence emission upon metal binding, yielding bi modal OFI/PET imaging tools for biomedical use. In conclusion, this doctoral project aimed to contribute to the advancement of sensing technologies for environmental monitoring and biomedical applications, highlighting the critical need for innovative solutions in the detection of new generations of pollutants, such as EPs, and for biomedical applications.

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OR51

A Key Cope-House Reaction Accomplishes the First Stereoselective Synthesis of Polyhydroxylated 3-Methylindolizidines

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Polyhydroxylated indolizidines, such as Castanospermine **1** (Figure 1a), with various substitution patterns, represent a deeply investigated class of iminosugars known for their biological activity (i.e. glycosidases inhibition, anticancer, antimetastatic, and antiviral activities).[1] However, related 5-methyl substituted indolizidines, such as Steviamine **2**, did not show interesting inhibitory activity.[2] On the other hand, naturally occurring polyhydroxylated pyrrolizidines – which can be considered as ring-contracted versions of indolizidines – with a methyl substituent adjacent to the bridge-head nitrogen atom, such as hyacinthacines A_3 **3** and B_3 **4**, inhibit intestinal lactase displaying antidiabetic activity.[1] This suggests a possible biological activity for indolizidines bearing a methyl substituent adjacent to nitrogen in the pyrrolidine moiety, which, however, have not been synthesized so far.

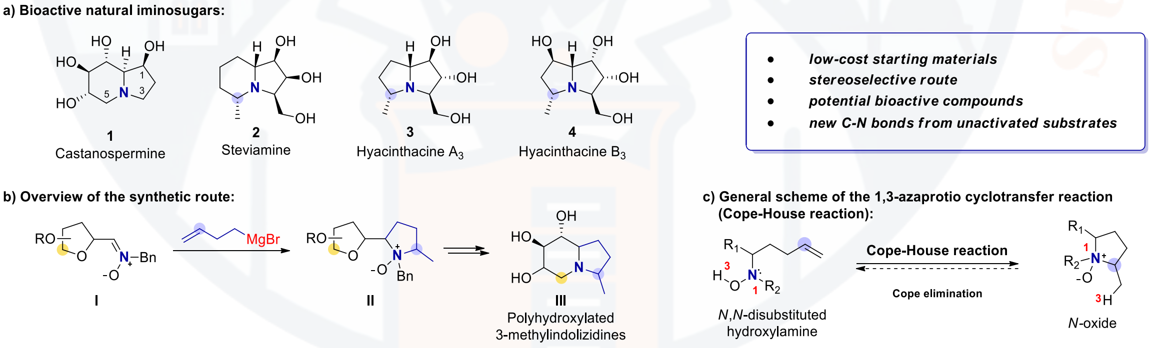

Figure 1: General overview of the work.

This work aims to present the first synthetic route to polyhydroxylated 3-methylindolizidines **III**, starting with enantiomerically pure nitrones **I** derived from low-cost sugars, and using the Cope-House reaction[3] as the key step for the construction of the key methyl pyrrolidine moiety **II** (Figure 1b and 1c). The biological activity of the final products is under evaluation.

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OR52

Synthesis and Application of Polynorepinephrine-Derived Biomimetic Receptors: Nanoparticles and Films for Advanced Biosensing

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A new generation of molecularly imprinted biopolymers derived from the endogenous neurotransmitter polynorepinephrine (MIPNEs) has been developed, highlighting their potential as versatile and cost-effective materials for protein recognition. A straightforward synthesis method produces films and nanoparticles imprinted with specific peptide sequences from target proteins through alkali-induced autoxidation of the monomer at low temperatures in aqueous media, resulting in three-dimensional recognition cavities capable of reversible and selective binding to the target protein. MIPNEs demonstrate significant promise as receptor mimics in bioanalytical affinity-based assays. These bioreceptors have been effectively integrated with various analytical techniques, including Surface Plasmon Resonance (SPR)[1] and Fiber-Optic Bio-Layer Interferometry (BLI),[2] achieving performance in human serum comparable to standard detection methods, using immunoglobulin G1 as the target. Similar outcomes are anticipated for MIPNE-based sensors targeting proteins such as human serum albumin (HSA) or myoglobin across diverse matrices. The versatility of MIPNEs has also enabled the development of innovative therapeutic tools. By harnessing their molecular recognition properties and biocompatibility, MIPNE NPs are being explored in biomedical applications as effective molecular catchers or drug delivery systems.[3] These results confirm the efficacy and flexibility of MIPNEs as biomimetic receptors, paving the way for their potential use as substitutes for antibodies.

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OR53

Anti-MOG glycopeptide antibodies for MOG antibody associated disease patient stratification

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Myelin oligodendrocyte glycoprotein antibody-associated disease (MOG-AD) is a rare inflammatory disease affecting the central nervous system. In MOG-AD, the immune system attacks myelin leading to symptoms such as vision loss, muscle weakness, stiffness or paralysis, confusion, seizures, and headaches, which can be confused with other diseases such as multiple sclerosis (MS) and neuromyelitis optica spectrum disorder (NMOSD). MOG-AD is characterized by the presence of anti-myelin-oligodendrocyte glycoprotein (MOG) antibodies, biomarkers of the disease.[1] Despite being the gold standard for detecting anti-MOG antibodies, cell-based assays have not yet been standardized, and reproducibility between testing centers has not been systematically investigated.[2] On the other hand, alternative peptide-based assays may offer several advantages: peptides can be site-specifically modified and efficiently produced by solid-phase synthetic approaches. This is relevant considering that aberrant post-translational modifications, particularly glycans, are involved in non-self immune recognition and could be linked to early misunderstood bacterial and/or viral infections, as a possible etiology. In this first year, peptides were designed and synthesized based on hMOG 25-55 (RISPGKNATGMEVGWYRPPFSRVVHLYRNGK), which includes the immunodominant fragment 35-55, the native glycosylation site N31. To study the role of glucosylation, the non-glucosylated sequence and the corresponding glucosylated analogs at positions N31, N53, and both were synthesized. All the synthetic peptides have been tested as synthetic antigenic probes in ELISA using sera samples from MOG-AD patients together with samples from MS and NMSOD patients. Also, the cross-reactivity with the hyperglucosylated nontypeable *Haemophilus influenzae* (NTHi) adhesin, which was previously shown to be connected to MS, has been investigated.[3] The results reported herein provide insight into MOG-AD patient stratification, based on differential immune responses, and the role of glycosylation and possibly early bacterial infection in the pathogenesis of MOG-AD.

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OR54

Design and applications of innovative polymeric materials

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In recent years, the social and environmental challenges linked to the exploitation of fossil resources have driven the search for more sustainable and eco-friendly alternatives. Among these, lignocellulosic materials stand out as one of the most significant natural sources for producing high-value-added materials and biopolymers. Their biodegradability, renewability, recyclability, and great availability make them highly appealing, particularly in the context of advancing eco-design principles.

This study explores strategies for lignocellulosic biomass valorisation to develop innovative materials for different applications within the manufacturing sector. One approach involves the production of biomaterials, such as composite panels or cellulose films, from the transformation of natural or waste fibres through pre-treatment processes and the solubilisation of the cellulosic fraction present in the biomass. Furthermore, starting from lignocellulosic feedstocks,[1] new polymer formulations can be designed by synthesizing biomonomers and biopolymers. Notably, biomonomers created from saccharides with polar and reactive functional groups can enhance the properties of final products while improving sustainability and recyclability. These biomonomers enable the synthesis of a variety of acrylic and vinyl copolymers by modulating their applicative properties. Experimental findings highlight the potential of these copolymers for their use in the development of advanced adhesives and other polymer systems, offering promising applications within eco-design frameworks.

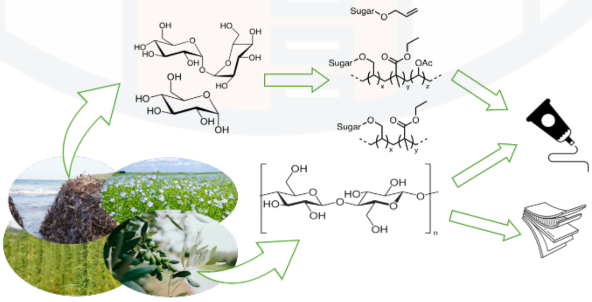

Figure 1: From biomass to new biomaterials.

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OR55

Gold nanoparticles and lipid vesicles: a gateway to advanced nanoplasmonic and SERS probes for biomedical applications

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Understanding the interactions at the nano-bio interface is crucial for developing innovative materials and technologies for biomedical applications.[1] In this context, recent studies showed that citrate-capped gold nanoparticles (AuNPs) spontaneously associate on the membrane of lipid vesicles, according to a membrane-templated process that combines the biocompatibility of lipids and the functional properties of AuNPs.[1-3] This contribution explores AuNPs-lipid membrane interactions aiming at: (i) probing ensemble-averaged properties of lipid membranes, by exploiting AuNP nanoplasmonics; (ii) designing novel and simple synthetic approaches for Surface Enhanced Raman Spectroscopy (SERS) tags.

First, AuNP nanoplasmonics was applied to characterize lipid vesicles, providing insights on the effect of membrane stiffness and concentration. By combining experimental techniques and numerical simulations, we introduce plasmonic isosbestic points as distinctive markers for the average interparticle spacing in plasmonic assemblies, allowing us to develop a colorimetric assay for quantifying membrane rigidity in biological samples with unknown concentration, such as extracellular vesicles (EVs).

Second, leveraging the spontaneous clustering of AuNPs on lipid bilayers, a simple hybrid platform ("LipoGold tags") was developed, using the lipid membrane as a scaffold to encapsulate hydrophobic Raman-active molecules (Raman Reporters, RRs) and induce AuNPs clustering, enhancing the electromagnetic field for SERS detection. LipoGold tags exhibited high colloidal stability, reproducibility, and adaptability across various RRs. Their functionalization with cellular probes enabled intracellular sensing, successfully detecting GM1 gangliosidosis alterations as a proof of concept. Overall, these findings highlight the potential of AuNP-lipid hybrid systems for biomedical applications, shedding light on the unexplored valence of isosbestic points in nanoplasmonics and introducing an accessible route to design efficient and versatile SERS probes.

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[2] L. Caselli et al., *Nanoscale Horiz.* **2021**, *6*, 543-550.
[3] J. Cardellini et al., *Nature Comm.* **2024**, *15*, 7975.

OR56

Study of the physico-chemical properties and hydration reactions of cement formulation based on ground granulated blast furnace slag with varying sulfate content

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The research focuses on investigating the physico-chemical properties of ternary cement formulations. These materials made of Portland cement, ground granulated blast furnace slag and inorganic fillers are one of the most promising alternatives to reduce greenhouse gas emissions by partially replacing Portland cement (the main contributor to CO_2 emissions during production) with supplementary cementitious materials. A series of physico-chemical analyses were carried out to identify the effect of sulfate in the ternary systems. Then, tests were carried out to understand water adsorption on the inorganic filler and its availability for hydration reactions. The hydration reactions were monitored using differential scanning calorimetry (DSC). DSC measurements were conducted to assess whether different sulfate contents in the mixture correspond to variations in hydration kinetics. The results obtained indicate that varying the sulfate amount within the cement mix impacts the characteristics of hydration kinetics. Moreover, isothermal calorimetry measurements were carried out to follow the hydration reactions. This technique allows us to measure heat flow associated with chemical reactions occurring during cement hydration.

Additionally, XRD analyses were conducted to evaluate the effect of changing the sulfate content in the mixture, particularly on the evolution of carboaluminates phases. Analyses on the inorganic filler were performed using thermogravimetric analysis (TGA) and DSC to determine the amount of water adsorbed on its surface and its availability for hydration reactions. The results showed that the adsorbed water is indeed available for hydration reactions. The future perspective will include rheological analyses to evaluate how sulfate can impact the rheology of this ternary blended cement and the inclusion of different types of sulfate sources.

OR57

Synthesis of iminosugar derivatives as potential agrochemicals for crop protection

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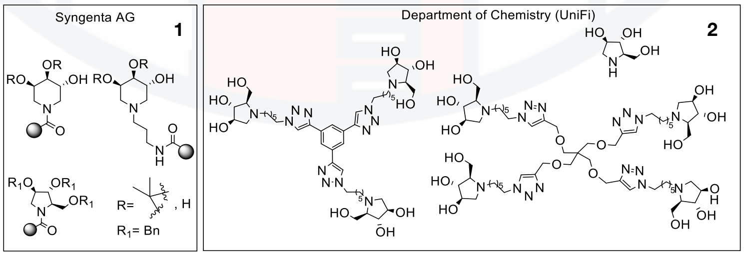
This project aims to develop safe, natural bactericides for crop protection, emphasizing non-toxic compounds with antibacterial and antifungal properties or targeted action against *Pseudomonas syringae*, employing iminosugars as the key functional agents. In collaboration with Syngenta AG, automated synthesis was employed to generate new small compounds libraries through amide coupling of piperidine or pyrrolidine iminosugar derivatives with various carboxylic acids from Syngenta's stock (**Figure 1**). The syntheses were performed in the company's automated laboratory, that greatly improves access to compounds' libraries and simplifies the investigation of their potential applications.[1] These compounds underwent systematic screening against multiple bacterial and fungal pathogens. At the Department of Chemistry (UniFi), our research further explored the synthesis of multimeric 1,4-deoxy-1,4-imine-D-arabinitol (**DAB-1**), derivatives (compounds **1** and **2**, **Figure 1**) to assess their potential as levansucrase inhibitors.[2] Levansucrase produces levan, a polymer essential for bacterial fitness and that might play a key role in the plant pathogen interaction during the early stages of infection.[3] In particular, in collaboration with the Department of Biomedical Sciences (UniFi), we proved that compounds **1** and **2** are potent inhibitors of levansucrase from *Pseudomonas syringae* pv. *actinidiae* (Psa), the causative agent of kiwifruit canker. Further investigation on their bactericidal activity is currently underway.



DAB-1

Figure 1: Iminosugar derivatives investigated as agrochemicals for crop protection.

[1] N. Collins et al., *Org. Proc. Res. Dev.* **2020**. *24*, 2064.
[2] C. Cicchi et al., *submitted.*
[3] S. Kasapis et al., *Carbohydr. Polym.* **1994**, *23*, 55-64.

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OR58

Electrodeposition and modification of surfaces of technological interest with low environmental impact

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The project aims to leverage the synergistic benefits of semiconductors and alloys through electrodeposition as a synthesis technique for spin-filtered photoelectrochemical water splitting and enhanced hydrogen production directly from solar energy. Its scope emphasizes applications in the 4.0 industry, environmental sustainability, metal recovery, and the optimization of industrial electrolytic processes. To achieve this goal, a thin film containing MnAs was successfully deposited via electrochemical methods, underscoring the critical role of electrochemistry in advancing spintronics and next-generation device development.[1] Furthermore, various nano- and microstructures of metals were electrodeposited on silicon substrates, and a customizable deposition procedure was developed to align with the specific requirements of final devices. These efforts provided valuable insights into optimizing industrial processes, particularly in electroplating plants, enhancing efficiency and scalability for large-scale applications.[2] The study also explored the potential of Metal-Assisted Chemical Etching (MACE) of doped silicon, starting from metal electrodeposition. This approach capitalizes on the advantages of electrodeposition, including scalability, speed, cost-effectiveness, and its ability to operate at room temperature and atmospheric pressure in aqueous solutions, enabling the synthesis of materials with tailored properties.[3] Voltammetric analyses were conducted using solutions containing Au and Ag to identify optimal electrochemical deposition conditions. Subsequently, the best etching parameters were determined to produce Silicon Nanowires (NWs) with the desired morphology and dimensions. These deposits and NWs were thoroughly characterized morphologically and compositionally using Scanning Electron Microscope (SEM) techniques. This procedure promises to develop compact, high-performance sensors and high-specific surface-area electrodes, particularly when NWs are further functionalized with metals or other chemical species. Additionally, an electrochemical cell was designed, engineered, and fabricated to evaluate the photoelectrochemical water-splitting performance of the electrodes produced during the study.

[1] G. Pappaianni et al., *J. Electrochem. Soc.* **2024**, *171*, 1-10.
[2] W. Giurlani et al., *Sustain.* **2024**, *16*, 1-31.
[3] A. Irrera et al., *Semicond. Sci. Technol.* **2017**, *32*, 1-20.

OR59

Technological and biological innovations in tackling Microplastics and Microfibers Pollution

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Microplastics (MPs) and microfibers (MFs) pollution, originating from plastic particles less than 5 mm in size, is a growing environmental concern that has permeated various ecosystems, from oceans and rivers to subterranean habitats. As global plastic production continues to rise, the fragmentation of larger plastic items and the direct release of MPs from industrial, domestic, and textile sources contribute to the widespread contamination of aquatic systems. The small size of these pollutants allows them to interact with a wide range of organisms and penetrate deep into environmental matrices, posing significant ecological and human health risks. Freshwater and groundwater environments, in particular, are critical conduits for plastic pollution, connecting terrestrial sources to marine sinks. Strong evidence of the predominance of MFs over other MPs types has been found by investigating the ingestion of these pollutants by meiofaunal taxa in urban streams (47%), by freshwater stingrays (64.7%), and in groundwater systems (80-95%). Traditional methods for MPs detection, such as visual identification and spectroscopic analysis, can be time-consuming and may not effectively capture MPs due to their small size. By combining high-resolution imaging with sophisticated data processing, automated particle analyzers can address these limitations, offering rapid, reproducible, and sensitive analyses capable of detecting fibers as small as 5 µm while providing detailed morphological data. Traditional remediation methods, such as incineration and recycling, have proven inadequate in addressing the scale of plastic waste, often generating secondary pollutants or suffering from economic and logistical challenges.[1,2] It is crucial to investigate alternative eco-friendly strategies to mitigate these MPs and MFs spreading. An efficient strategy for MFs remediation has been found in magnetic micro/nanoparticles that achieved high removal rates, with efficiencies surpassing 80% under optimized conditions. Another promising approach is bioremediation, which exploits microbial metabolism to degrade complex polymers. In this context, a novel bacterium capable of degrading low-density polyethylene has been identified and characterized.

[1] OECD, Policy scenarios for eliminating plastic pollution by 2040, **2024**.
[2] P. Pandey et al., *Waste Disp. & Sust. En.* **2023**, 1-18.

OR60

Targeting Intrinsically Disordered Proteins in Neurodegenerative Diseases: Exploring pharmacological chaperone for Dual Action on α-Synuclein and GCase

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Intrinsically disordered proteins (IDPs) are highly flexible molecules often linked to the onset of incurable diseases. Despite their great therapeutic potential, IDPs are often considered as undruggable because they lack defined binding pockets, at the basis of drug discovery approaches. However, small molecules that interact with the intrinsically disordered state of α-synuclein, the protein linked to Parkinson’s disease (PD), were recently identified and shown to act as chemical chaperones (CC).[1] Glucocerebrosidase (GCase) is an enzyme crucially involved in PD, since mutations that code for GCase are among the most frequent genetic risk factors for PD.[2] Following the “dual-target” approach, stating that one carefully designed molecule can in principle interfere with more than one target, we identified a pharmacological chaperone for GCase that interacts with the intrinsically disordered monomeric form of α-synuclein (α-syn).

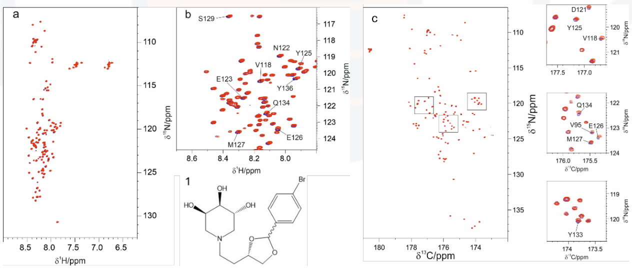

Figure 1: NMR monitoring of α-syn interaction with CC (panel 1). (A) HSQC ^{1}H-^{15}N spectra overlay: α-syn alone (blue) vs. with CC (red). (B) Enlarged view of regions with significant chemical shift perturbations. (C) CON spectra overlay: α-syn alone (blue) vs. with CC (red), with three zoomed-in regions

[1] P. Robustelli et al., *J. Am. Chem. Soc.* **2022**, *144*, 2501-2510.
[2] A. D. Klein et al., *Nat. Commun.* **2023**, *14*, 6383.

OR61

Eco-Friendly Optoelectronic Devices: Semiconductors and Solar Cells for a Cleaner Tomorrow

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In recent decades, there have been significant improvements in the performance of chalcogenide thin-film solar cells. However, these technologies rely on costly, toxic, and scarce elements such as cadmium, tellurium, and indium, which present both environmental and economic challenges. In this regard, Cu_2ZnSnS_4 (CZTS) stands out as a highly promising inorganic semiconductor for low-cost thin-film photovoltaic devices, as it is made from abundant, inexpensive, non-toxic, and readily available elements. An innovative low-temperature synthetic pathway was developed to produce Cu_2ZnSnS_4 nanoparticles, which were extensively characterized through various techniques (HR-TEM, XPS, EDX, ICP, and Micro-Raman spectroscopy, EPR, SQUID magnetometry, and MCD). Nanoparticles were then employed to fabricate CZTS-based solar cells, using both a classical bilayer architecture as well as hybrid organic-inorganic solar cells. An innovative and innovative semiconducting molecular system has also been studied in parallel to CZTS-based systems. These molecular materials potentially relevant for application in optoelectronic and magnetism fields were deposited in high vacuum using thermal sublimation. The thin films that were produced were studied through XPS and AFM, moreover, an extensive structural investigation was conducted at the Diamond Light Source, while the electric properties of the molecular assemblies were evaluated by performing J-V scans with an in-house setup recently developed in our labs.

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Comparative Evaluations of Thermochemical Reactions for Residual Biomass Conversion

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Biorefineries represent an industrial strategy for the valorization of biomass, providing value-added products, typically comprising a complex integrated network of physical and chemical transformation processes, such as mechanical and physical biomass pre-treatment, thermochemical (e.g. pyrolysis, gasification), catalytic and enzymatic reactions, and downstream purification processes. In this context, thermochemical processes (pyrolysis[1] and hydrothermal liquefaction[2]) are the most versatile conversion reactions, since they can transform feedstocks with heterogeneous compositions under the same operating conditions. In this research, thermochemical reactions were performed on two residual biomasses: the fibrous spheres of Posidonia Oceanica that annually accumulate along the coastline and an original industrial biowaste consisting of a spent herbaceous mixture from the agricultural industry. Firstly, a parallel analysis of two different heating technologies for slow pyrolysis was examined, comparing microwave heating (MAP) and conventional heating. The results showed that microwave pyrolysis generally results in a more extensive decomposition of the feedstock, while the use of conventional pyrolysis allows the collection of the first degradation products of the holocellulose fraction (levoglucosan) as well as substituted phenols. Furthermore, the use of the microwave absorber in the case of MAP influences the products distribution, promoting the non-condensable phase. In general, pyrolysis is particularly successful for the production of bio-char in addition to the production of syngas. Alternatively, the conversion of biomass by an alternative thermochemical reaction such as hydrothermal liquefaction, using water in the subcritical phase, maximizes the yield of liquid products. These products also exhibit a different composition compared to the condensable fractions of pyrolysis containing more long-chain fatty acids and substituted phenols. The analysis of these collected data reveals that the use of different conversion reactions directs the biomass valorization process towards specific reaction products and modulates their chemical-physical composition.

[1] R. Gallorini et al., *J. Anal. Appl. Pyrolysis* **2023**, *174*, 106138.
[2] A.R.K. Gollakota et al., *Renew. Sust. Energ. Rev.* **2018**, *81*, 1378-1392.

OR63

Antibody-drug conjugates: a strategy of purification and identification

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Antibody-drug conjugates (ADCs) are powerful tools. They have demonstrated remarkable selectivity and cytotoxicity, able to target with precision cells, driven by advances in monoclonal antibody (mAb) technologies.[1] The global mAb market, valued at USD 162 billion in 2021, is projected to continue its growth, with oncology treatments constituting a significant portion.[2,3] ADCs present structural and functional challenges due to the inherent heterogeneity of mAbs caused by post-translational modifications (PTMs), combined with the variability introduced by conjugation strategies, linker properties, and payload characteristics. These factors necessitate robust methodologies for ADC characterization and purification, leveraging analytical techniques to evaluate their structure, conjugation profiles, and physicochemical properties. This study focused on developing a two-step protocol for ADC synthesis, optimizing the process with three model antibodies (Rituximab, Matuzumab, and Trastuzumab) conjugated to polyarginine peptides using the s-SMCC linker. Analytical characterization employed various chromatography techniques, including Hydrophobic Interaction Chromatography (HIC), Weak Cation Exchange Chromatography (WCX), Size Exclusion Chromatography (SEC), and Reverse Phase Liquid Chromatography (RP-LC), with optimization of operational parameters such as buffers, gradients, and temperature. Initial results showed mixed outcomes; WCX demonstrated promising separation performance, while challenges in HIC and SEC indicated further refinement is needed. Additionally, a novel solid support (Eshmuno® CMX resin) combining HIC and WCX properties, was explored. The work established a foundation for ADC synthesis and characterization, forming the basis for future research to integrate these chromatographic techniques into a multi-dimensional liquid chromatography (mD-LC) workflow. Subsequent efforts will focus on coupling these methods with High-Resolution Mass Spectrometry (HR-MS) to enable continuous purification and comprehensive characterization of ADCs, advancing the development of precision oncology therapeutics.

[1] Y. J. Matsuda, *Sep. Sci*. **2022**, *45(1)*, 27-37.
[2] H. Kaplon, **2022**, *14(1)*, 2014296.
[3] H. Chen, *Molecules*, **2017** 1, *22(8)*, 1281.

OR64

Development of hybrid devices based on a liquid metal alloy junction

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Though challenging and delicate to handle, hybrid architectures containing molecular systems hold great promise for developing innovative devices. These systems offer unique functionalities, enabling selective electron transmission and transport. By integrating molecular components into inorganic device designs, such architectures open exciting prospects for advancements in spintronics, information processing, and other cutting-edge technologies.[1] A setup based on the use of a soft electrode such as eutectic gallium-indium (EGaIn, schematized in Figure 1) was developed and optimized as a gentle and versatile probe, capable of operating under an externally applied magnetic field to investigate electric transport properties in a vertical geometry. The liquid metal alloy forms soft, conformal junctions with the surfaces under investigation, minimizing damage while maintaining stable electrical contact.[2] With a junction area characterized by a radius on the order of tens of microns, the EGaIn setup enables studies at scales significantly larger than those probed by conductive-tip atomic force microscopy, approaching dimensions relevant to practical devices. Preliminary measurements were conducted on self-assembled monolayers of thiols ($C_{12}SH$) on template-stripped gold (Au^{TS}), yielding values consistent with those reported in the literature,[2] thereby validating the setup's reliability. Additional experiments were performed on a 100 nm thick film of the paramagnetic hydrogen-free [$Cu(dttt)_2$] molecule (1,3,2-dithiazole-4-thione-5-thiolate, $dttt^-$)[3] deposited on indium tin oxide via physical vapor deposition. The measured current-voltage characteristics of this system suggest memristive behavior, offering intriguing prospects for further exploration of its potential in memory and neuromorphic devices.

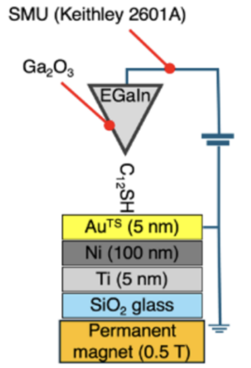

Figure 1: A junction probed under an applied magnetic field.

[1] E. Coronado, *Nat. Rev. Mater.* **2020**, *5*, 87-104.
[2] C. Nijhuis, et al., *J. Am. Chem. Soc.* **2009**, *131*, 17814-17827.
[3] F. Santanni et al., *JACS Au*, **2023**, *3*, 1250-1262.

OR65

Advanced spectroscopic study aiming to the understanding of the heme biosynthetic pathway of Gram-positive bacteria

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Heme *b* porphyrin is essential for bacterial pathogens to survive and infect the host. Unlike humans, monoderm bacteria produce heme *b* via the coproporphyrin-dependent (CPD) biosynthesis pathway [1]. In the penultimate step of the CPD route, the key enzyme coproporphyrin ferrochelatase (CpfC) catalyses the insertion of ferrous iron into coproporphyrin III (cpIII) producing ferric coproheme. Afterwards, the decarboxylase enzyme generates heme *b* by a two-step oxidative decarboxylation of the coproheme propionate groups at positions 2 and 4 to vinyl groups, in the presence of H_2O_2.[1]
Here I will highlight the most important accomplishments I achieved on the study of the active site of CpfC from Firmicutes *Listeria monocytogenes* (*Lm*CpfC) and Actinobacterium *Corynebacterium diphtheriae* (*Cd*CpfC) by UV-vis and resonance Raman spectroscopies using the physiological substrate (cpIII) and product (coproheme). The characterization of the native proteins and site-directed variants, targeting active site crucial residues, revealed that the H-bonding interactions between polar amino acids and porphyrin propionates are fundamental for correct binding and stabilization within the protein pocket.[2] The ferrous iron titration *in vitro* of cpIII demonstrated the formation of a ferric saddle-distorted intermediate reaction species as a consequence of the readjustment of the propionates H-bonds upon metalation.[3] Finally, I identified the metal access channel to the active site by using an exogenous model ligand. Unlike *Lm*, *Cd*CpfC contains a $[2Fe\text{-}2S]^{2+}$ cluster whose role is still under debate. The assignment of the bridging and terminal FeS stretching vibrations allowed us to disclose the type and configuration of the cluster's ligands in solution. Studying a variant without the cluster revealed its crucial role in maintaining the structural integrity of the active site and enzyme functionality. The understanding at the molecular level of the structure-function relationship in ferrochelatases from antibiotic-resistant bacterial pathogens is essential for developing mechanism-based therapeutic drugs.

[1] H.A. Dailey et al., *Proc. Natl. Acad. Sci. USA*, **2015**, *112*, 2210-15.
[2] A. Dali et al., *Protein Sci.*, **2023**, *32*, e4534.
[3] T. Gabler et al., *Protein Sci.*, **2023**, *32*, e4788.

OR66

PFAS removal by using graphene-polymer nanosheets

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Per- and polyfluoroalkyl substances (PFAS) including perfluorooctanoic acid and perflurooctanesulfonic acid (PFOS), are persistent pollutants posing significant environmental and health challenges due to their resistance in environment.[1] The issue of PFAS in water bodies is a pressing problem linked not only to long-chain molecules but, above all, to the introduction of short-chain compounds, which represent the most critical concern. This study evaluates the potential of a novel nanocomposite of graphene nanosheets, chitosan polymer, and zinc oxide (ZnO) for PFAS removal from water. Chitosan, a biodegradable polymer with functional amine and hydroxyl groups, exhibits limited adsorption capacity when used alone.[2] However, incorporation of the ZnO nanoparticles and of graphene nanosheet is expected to lead to a porous and hydrophilic composite with a more to efficient PFAS adsorption capability.

Batch experiments provided crucial insights into adsorption kinetics and isotherms, revealing that the ZnO-chitosan composite achieved higher adsorption capacities within shorter contact times. This enhanced performance is presumed to be due to increased surface functionality and electron transfer potential offered by ZnO and graphene nanosheets, enhancing stronger interactions with PFAS molecules. In addition, the hydrophilic character of the composite imparted by chitosan improved its water compatibility, ensuring effective dispersion and accessibility of active sites.

Preliminary batch adsorption studies exhibited a better removal percentage with the ZnO-chitosan-graphene composite than chitosan alone. The Transmission Electron Microscopy (TEM) revealed well-dispersed nanostructures, correlating with improved adsorption kinetics and capacities. This enhancement is due to the composite's increased active sites with much stronger interaction energies with PFAS molecules and greater water compatibility. The results also signified that ZnO-chitosan-graphene composites could become promising adsorbents for the effective remediation of PFAS pollutants in water. This approach offers a scalable and sustainable solution for water treatment. Further studies will assess the reusability and efficient use of the material in complex conditions.[3]

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[2] R. Ikram et al., *Polymers.* **2021**, *19*, 3266-3275.
[3] A. Samadi et al., *Chem. Eng. J.* **2023.** *14756.*

OR67

Design and Development of Wearable Electrochemical Sensor for The Monitoring of Clinical Parameters

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Wearable sensors have emerged as a powerful tool in the medical device field, offering significant advantages over conventional devices used for diagnosis and monitoring of medical treatments. These sensors integrate seamlessly into patients' daily lives and can utilize peripheral biofluids, reducing the impact on patient compliance and mental well-being. Moreover, they offer the possibility to use peripheral biofluids further minimizes the burden on patients, as previously mentioned. Furthermore, wearables open a new scenario in the field of the "Next Generation Digital Biomarkers", also defined as potential biomarkers related to a pathology, that are accessible in peripheral biofluids in a continuous manner; thus, they can be easily measured. Concerning this purpose, electrochemical sensors are particularly suited for the detection of biomarkers and the conversion of the signal from chemical to digital one.

The main goal of this thesis is the development of electrochemical sensors capable of detecting analytes for diagnostic and/or theragnostic purposes and converting the chemical signal into a digitalized one. To achieve wearable biocompatible electrochemical sensor, screen-printed electrodes have been chosen due to their peculiar properties such as flexibility, adaptability to different supports, and low-cost production. Moreover, the surface of such electrodes can undergo a plethora of modifications that assure an increase in terms of reproducibility, sensitivity, and stability, including chemical modifications, nanostructuration, physical treatments, etc. Each modification step was characterized using reversible, well-known, redox probe and evaluated with specific analyte in standard solutions and in artificial biofluids. The study also explored the sensor's behavior under conditions simulating real-life scenario, such as the presence of interfering species and matrix effects with the aim to maintain high performances in real samples further applications.

OR68

Hofmeister Effects on the Gelation Properties of a Peptide Hydrogel

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Peptide gels represent a versatile platform for the design of multi-responsive materials with customizable properties. Advances in solid-phase peptide synthesis (SPPS) largely improved the exploration of these systems. However, a frequently overlooked aspect is post-synthesis residual electrolytes such as trifluoroacetate ($TFAc^-$) which significantly impact the system properties.

A thorough understanding of ion behavior remains crucial to gain insights into complex systems [1,2]. In this study we investigated 3% w/v ACP(65-74)-NH_2 peptide hydrogels in the presence of different counterions: $TFAc^-$, SO_4^{2-}, Cl^-, Br^-, and I^-.

Our results show that the nature of the counterion influences the gelation properties, morphology and rheological properties (See Figure 1). We correlate these experimental findings with some ion-specific physicochemical parameters and conformational data, emphasizing the intricate effects of ion-peptide interactions and hydration.

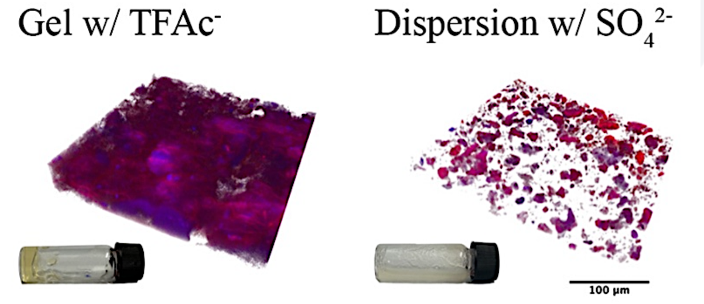

Figure 1: Confocal Laser Scanning Microscopy 3D reconstructions of 3% w/v ACP(65-74)-NH_2 hydrogels showing morphological differences: a gel structure with $TFAc^-$ counterions and a dispersion with SO_4^{2-} counterions.

[1] P. Lo Nostro et al., *Chem. Rev.* **2012**, *112*, 2286.
[2] M. Acar et al., *Colloids Surf. B*, **2024**, *236*, 113789.

OR69

Electrochemical Urea Sensing in Wastewater Using a Flow Biocatalytic Approach

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The timely assessment of urea levels in water and wastewater is essential for mitigating pollution and advancing remediation strategies, including processes that convert urea into valuable energy resources.[1] This research introduces a tailored potentiometric platform based on urease for detecting urea in wastewater samples. The system employs amino-functionalized glass beads as a support matrix for immobilizing urease in a custom-built bioreactor. Through an online flow measurement setup, the NH_4^+ generated by the enzymatic reaction was quantified using a potentiometric sensor placed in a specialized flow cell.

Key operational and analytical parameters were fine-tuned to optimize bioreactor efficiency. A detailed analysis of the buffer composition was performed to evaluate its impact on sensitivity and detection limits, highlighting the necessity of adjusting buffer concentration according to the sample type (LOD 8.93×10^{-6} M). Once optimized, the system was tested on spiked wastewater samples, employing the standard addition method to achieve an average recovery rate of 102 ± 5%. Despite the presence of interferents, these results demonstrate the feasibility of using the developed platform for remote, real-time monitoring of urea in wastewater.

An alternative method for urea quantification, based on an amperometric technique, is currently under development. This approach utilizes nickel nanomaterial-based electrodes for enhanced performance.

[1] W. Yan et al., *Appl. Catal. B: Environ.* **2012**, *127*, 221-226.

OR70

Dextran-Modified Poly(allylamine) Nanoparticles as Nanocarriers for the Delivery of Enzymes involved in Lysosomal Storage Diseases

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Lysosomal storage diseases (LSDs) are rare inherited disorders caused by defects in lysosomal enzymes, resulting in the accumulation of undegraded macromolecules and progressive tissue damage.[1] Enzyme replacement therapy (ERT) has emerged as a standard treatment for several LSDs, such as the Hunter's syndrome for which the recombinant human enzyme idursulfase (Elaprase®) is given by intravenous infusion.[2] However, the delivery of these therapeutic enzymes remains challenging due to poor stability, rapid degradation, and limited cellular uptake. To overcome these challenges, smart nanosystems offer a promising solution by protecting enzymes and facilitating their targeted delivery to lysosomes. Poly(allylamine) hydrochloride (PAH) are polymers that self-assemble into nanoparticles in phosphate buffer (PB) and have been investigated for their pH-responsive properties.[3] However, their positive charge can cause toxicity at high concentrations, requiring modifications for improved biocompatibility. In this study, dextran (DEX) with two different molecular weights (6 KDa and 9-11 KDa) was conjugated into the PAH backbone resulting in the formation of glyconanoparticles (glyco-NPs) in PB. In addition to improve the biocompatibility of the NPs, DEX should guarantee efficient intracellular uptake, and thus cargo delivery to cells. After physico-chemical characterization (NMR, DLS, cryo-EM), the potential of these glyco-NPs as delivery systems was evaluated using bovine serum albumin (BSA) as a model protein. The pH-dependent BSA encapsulation and release was demonstrated with different complementary methods (FCS, CD, DLS, BCA). The encapsulation and delivery of idursulfase (provided by Prof. Amelia Morrone from Meyer Children's Hospital IRCCS, Firenze) is currently under investigation. These studies focus on optimizing the release profile of idursulfase and assessing the efficacy of smart glyco-NPs compared to non-encapsulated idursulfase, towards a new delivery system for the potential treatment of Hunter's disease.

[1] F. M. Platt et al., *Nat Rev Dis Primers.* **2018**, *4*, 27.
[2] M. Stapleton et al., *Expert Opin Orphan Drugs*. **2017**, *5*, 295-307.
[3] P. Andreozzi et al., *Appl. Mater. Interfaces*. **2017**, *9*, 38242-38254.

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OR71

Study of new eco-friendly materials for Cultural Heritage preservation

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The conservation of Cultural Heritage materials, particularly wood and stone, requires advanced protective treatments that ensure long-term preservation while respecting environmental and regulatory constraints. This research focuses on the synthesis and application of oligoamides and amines functionalized with short fluorinated hydrophobic pendants to impart superior resistance to water and other environmental stressors.[1] These novel formulations aim to protect wood and stone artifacts without altering their aesthetic or structural integrity while also reducing the risks of environmental impact. Fluorinated derivatives were synthesized and applied using eco-friendly solvents and their formulations were optimized to improve performance. Their evaluation, through diagnostic protocols such as water (WCA) and oil (OCA) contact angle measurements, chromaticity analysis, and stress testing, has demonstrated excellent hydrophobic and oleophobic properties, coupled with durability under UV radiation and mechanical mild abrasion. To enhance the protection ability of the formulations against light, these compounds have been combined with advanced light stabilizers, including Hindered Amine Light Stabilizers (HALS) and Ultraviolet Light Absorbers (UVA).[2] An in-dept study of the long-term degradation of the achieved coatings was carried out through spectroscopic techniques. In light of the environmental and regulatory challenges related to PFAS (Per- and Polyfluoroalkyl Substances), this study also envisaged the development of fluorine-free protective agents. These new materials provide eco-friendly alternatives without compromising hydrophobic performance. Preliminary comparative studies confirmed that these formulations are promising in preserving both wood and stone artifacts. For the removal of surface coatings obtained with the studied protective products new organogels were designed to facilitate the confinement of the removed materials.[3] These gel systems, tailored with advanced thickeners and crosslinkers, facilitate the controlled removal of aged coatings and residues while minimizing solvent usage and safeguarding the integrity of underlying substrates. These findings contribute to the development of durable, sustainable, and environmentally compliant solutions for safeguarding cultural artifacts, ensuring their longevity for future generations.

[1] Y. Zhang et al., *Coatings*, **2022**, *927*, 1-25.
[2] M. Pánek et al., *Materials*, **2021**, *189*, 109600.
[3] N. Khaksar-Baghan et al., *Herit. Sci.* **2024**, *12* (1), 248.

OR72

Multivalent Golgi-targeting compounds for the precision delivery of cancer therapeutics

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The precise delivery of drugs to cancer cells is crucial for the development of therapeutics enhancing specificity and efficacy, while minimizing off-target effects. All cells are coated by complex carbohydrates (glycans), and alterations in the structure and occurrence of glycans is linked to cancer hallmarks.[1] Golgi apparatus (GA)-resident glycosyltransferases (GTs) are enzymes that regulate glycan synthesis and thus are potential targets for treating cancer, as the selective modulation of their activity gives the opportunity to custom modify the glycocalyx on the surface of cancer cells. A few GA-targeting probes have been reported so far, and most of them are fluorescent markers for subcellular labeling.[2] It has also been found that a multivalent display of these molecules can significantly improve their Golgi targeting ability.[3] Therefore, this project focuses on the identification of GA-targeting moieties, their multimerization into suitable scaffolds, and further conjugation to a BODIPY-based fluorescent tag in order to track their intracellular fate. In this way, a systematic study for the selection of the most effective GA-targeting moieties is being carried out. The further conjugation of the selected multivalent compounds will open the way to the precision subcellular delivery of GTs modulators to improve their therapeutic effect.

[1] S. Pinho et al., *Nat. Rev*. **2015**, *15*, 540-555
[2] Wang et al., *Coord. Chem. Rev.* **2024**, 502, 215618.
[3] R.S. Li et al., *Chem. Sci.* **2017**, *8*, 6829-6835

Acknowlegment: This work has received funding from the European Union's Horizon Europe research and innovation programme under the Marie Skłodowska-Curie Actions Grant Agreement n. 101119601 (GLYCANDRUG)"

OR73

Shedding light on the electron delocalization pathway at the $[Fe_2S_2]^{2+}$ cluster of FDX2

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In this manuscript we investigate the electronic structure of the $[Fe_2S_2]^{2+}$ cluster of human ferredoxin 2 by designing NMR experiments tailored to observe the hyperfine-shifted and fast relaxing resonances in the immediate proximity of the cluster, and adding a quantitative layer of interpretation through quantum chemical calculations. The combination of paramagnetic NMR[1-3] and density functional theory data provides evidences on the way unpaired electron density map is at the origin of the in-equivalence of the two iron(III) ferredoxin centers. An electron spin density transfer is observed between cluster inorgan-ic sulfide ions and aliphatic carbon atoms, occurring via a C-H---S-Fe^{3+} interaction, suggesting that inorganic cluster sulfide ions have a significant role in determining the coordination sphere of the prosthetic group. Extended assignment of ^{1}H, ^{13}C and ^{15}N nuclei allows to identify all residues of the binding loop and provides an estimate of the magnetic exchange coupling constant among the $[Fe_2S_2]^{2+}$ cluster of 386 cm^{-1}. The approach developed here can be extended to other iron-sulfur pro-teins, providing a crucial tool to uncover the subtle differences in electronic structures that modulate the functions of this protein family.

[1] K. Cai el al., *Biochemistry* **2017**, *56 (3)*, 487-499.
[2] Machonkin et al., *J. Am. Chem. Soc.* **2004**, *126 (17)*, 5413-26.
[3] S. Ciofi-Baffoni et al., *J. Biomol. NMR* **2014**, *58 (2)*, 123-8.

OR74

Optimising Biochar-Based Column Filtration Systems for Enhanced Pollutant Removal in Wastewater Treatment: A Preliminary Study

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This research aims to optimise wastewater treatment using lab-scale biochar-based column filtration systems (CFSs) as a preliminary study to design larger scale filters such as constructed wetlands. This study focuses on two sub-studies. Sub-study 1 aims to optimise the percentage of BC (0%, 10%, 25%, and 50%) in filling medium of CFSs, by performing lab-scale column tests on decanted wastewater for 5 months. The BC used here was produced from olive pomace (OP) pyrolysed at 590 °C for 2 h and at a heating rate of 10 °C min^{-1}. Sub-study 3 aims to test the treatment performance of CFSs integrated with BCs from OP (CFS-BOP), orange waste (CFS-BOW), filao (CFS-BF), and cypress (CFS-BCY). The production of OP-derived BC is described in sub-study 2. BCs other than BC-OP were produced at a heating rate of 2 °C min^{-1} up to 400 °C for 12 h. The results of sub-study 1 revealed that the BC incorporated into the CFSs improved the efficiency of nitrogen species removal (total nitrogen, TN 64% - 65%; organic nitrogen 78% - 87%; NH_4^+-N 57% - 69%), phosphorus species (total phosphorus, TP 39% - 44%; PO_4^{3-} 38% - 42%), total and soluble chemical oxygen demand (TCOD 44% - 56%; SCOD 33% - 51%), and total suspended solids (TSS 87% - 92%), compared to CFS0. The bacteriological analysis includes faecal indicators and pathogens. Furthermore, the highest removal efficiencies were observed for CFS10. The results of the sub-study 2 showed that biochar-based CFS provided higher removal efficiencies for TN, NH_4^+-N, TCOD, and absorbance (ABS 254 and 420 nm). Notably, CFS-BOW has the best removal rates compared to CFS0 for TN (45% vs. 27%), NH_4^+-N (87% vs. 78%), COD (63% vs. 47%), and ABS 254 nm (40% vs. 34%). The higher removal of NH_4^+-N was accompanied by a high release of nitrate (NO_3^--N) due to nitrification. No significant effect of biochar integration was observed for phosphorus removal. In addition, biochar-based CFS showed higher removal of bacteriological indicators, such as total coliform, faecal coliform, and faecal streptococci, compared to the control filter.

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POS01

Formulation and Physicochemical Characterization of Self-Assembling Biomolecular Aggregates and "Green" Sustainable Microcapsules

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The research project focuses on the formulation and physicochemical characterization of self-assembling aggregates of surfactants, macromolecules, and microcapsules derived from bio-based compounds (e.g., plant resins), stabilized by bio-derived surfactants obtained from sustainable waste materials. The characterization involves techniques such as light and X-ray scattering, microscopy (electron, confocal, IR, and Raman), and thermal analysis (DSC, DTG). The goal is to characterize the structure and dynamics of these self-assembling systems and to assess their potential applications in fields ranging from cultural heritage preservation to cosmetics and textile industry.

The first focus is on fibroin-based systems for the consolidation of silk and other textile artifacts, aiming to develop a sustainable prototype using renewable materials. Fibroin and cellulose nanocrystals (CNC) are ideal consolidants compatible with fibers. A hybrid SRSF (self-regenerated silk fibroin)-CNC formulation has been obtained starting from silk textile waste,[1,2] and characterized by studying its self-assembly, rheological behavior, and the secondary structure of films formed by casting. Tests on aged silk fibers also demonstrated its superior consolidating effect compared to pure SRSF or CNC. However, while CNC enhances mechanical properties, it also accelerates fibroin self-assembly, significantly lowering the formulation's shelf-life. Thus, new SRSF-CNC formulations with bio-derived additives (arginine, sericine) are now being explored, and thoroughly characterized, to control self-assembly and aggregation.

The second focus is on the development of sustainable microencapsulation of actives like perfumed raw materials (PRMs) in water-based systems for home and personal care products.[3] The research will explore the use of natural resins and glycerol-derived surfactants to create sustainable bio-based capsules, controlling their size and actives' release to enhance their performance and promote an eco-friendlier approach. Potential impact is to all sectors where controlled encapsulation and delivery of actives are fundamental (drug-delivery, food industry, agriculture, detergency, textiles, etc.).

[1] C. Cianci et al., *Colloids Surf. A: Physicochem. Eng. Asp*. **2022**, *634*, 127944.
[2] D. Chelazzi et al., *Journ. of Coll. and Interf. Sc.* **2020**, *576*, 230-240.
[3] M. Mamusa et al., *Angewandte Chemie Intern. Edit.* **2021**, *60.44*, 23849-23857.

POS02

Synthesis of paramagnetic porphyrin-based complexes and preliminary measurements for optical spin polarization

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A challenge in QI (quantum information), is represented by the necessity of initializing a qubit in a well-defined computational state. Focusing on molecular electron-spin based systems, such a condition can be achieved by applying a magnetic field; however, given the small Zeeman energy gap, such a mechanism is only operative at *sub-kelvin* temperatures. More recently, a promising approach has been proposed involving light driven processes on ancillary chromophores[1]. Beyond the chemical versatility in accommodating the construction of multi-qubit architectures, the conjugated structure of porphyrins is responsible for great light absorption in the visible region, making these systems the perfect candidates for the study of light-induced qubit's initialization[2].
By taking advantage of synthetic chemistry, this project aims to tune the exchange and dipolar interactions in porphyrin-based dimers (Figure 1), looking for the best compromise in terms of coupling regime, and satisfying both spin addressability and multi-qubit implementation[3].

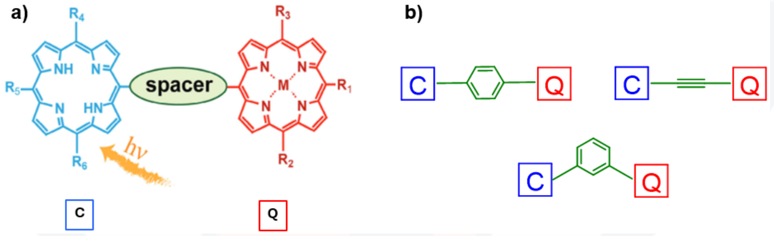

Figure 1: a) [C-Q] (chromophore-qubit) dimer system; b) Proposed spacers for exchange coupling interaction tuning.

The outcoming knowledge in the regard of the optimization of the spacer's nature and exchange coupling magnitude will be exploited at a later stage for the investigation of more complex architectures, *i.e.*, systems in which the molecular qubit Q is connected to a donor-acceptor dyads in the presence of chiral media, to observe spin selective light driven processes, *i.e.,* CISS effect.

[1] H. Mao et al., *J. Phys. Chem. B*, **2022**, *126*, 10519-10527.
[2] A. Privitera et al., *J. Am. Chem. Soc.* in press (arXiv:2408.02104).
[3] D. Ranieri et al., *Angew. Chem. Int. Ed.* **2023**, *62,* e202312936.

POS03

Use of Sergent & Soldiers effect for chirality control of supramolecular nanotubes of Single-Chain Magnets deposition

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Single-Chain Magnets are monodimensional compounds showing magnetic retention of the magnetization, a behaviour suitable for data storage purposes. Unfortunately, deposition issues restrain the advances in this way. Recently, a type of SCMs based on nitronyl-nitroxide radical coordinated to Tb^{3+} ions have shown a peculiar nanotube organization.[1] These nanotubes, in specific conditions (figure 1), show a metallogel structure allowing to deposit them on different substrate.[2] To reach a better control of the deposition, chiral nanotubes were synthesized thanks to Sergent & Soldiers effect. Herein, we describe the synthesis, characterization and deposition of Sergent & Soldiers compounds based on (R) and (S)-2-(4'-(octadecyloxy)phenyl)-4,4,5,5-tetra-methylimidazolin-1-oxyl-3-oxide) (NIT-C_{18}(R/S)) based Tb(III) chains. These chains showed SCM magnetic properties and chiral supramolecular organization evidenced by CD measurements. Thus, it appears as an interesting way of controlling all parameters of these supramolecular nanotubes on surface.

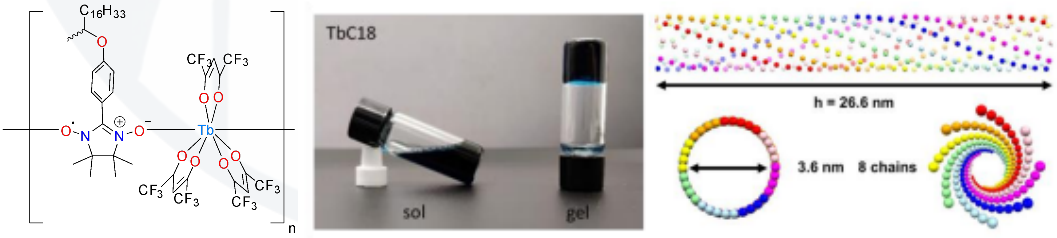

Figure 1: TbNIT-C18 chain (left), gelation test of TbNIT-C18 (middle) and representation of the supramolecular nanotube extracted from SAXS measurements of TbNIT-C18 gel.

[1] F. Houard et al. *Angew. Chem*. **2020**, *59*, 780.
[2] F. Houard et al. *Mater. Horiz.* **2023**, *10*, 547.

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POS04

Nanocellulose as biocompatible and versatile platform for delivering drugs

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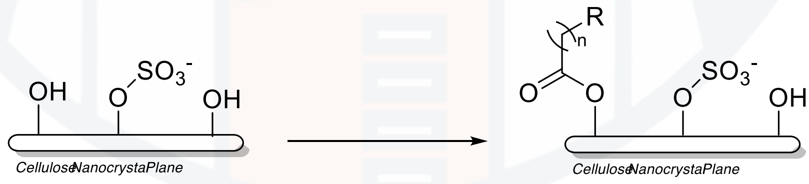
Cellulosic nanomaterials, originated from renewable sources, represent a promising, but not yet fully explored, platform for biomedical applications,[1] ranging from classical drug-delivery systems to the formation of bio-active surfaces and 3D devices. Nanocellulose's structure and dimensions are responsible for its good dispersibility in aqueous solutions and the ability to accumulate within the cell space, even if functionalized.[2] This reason makes nanocellulose an ideal candidate for drug transport. In this project, the goal is to functionalize crystalline nanocellulose with bioactive molecules such as Auranofin, Curcumin, and 5-fluorouracil prodrugs. Two approaches could lead to the adhesion of these bioactive molecules onto nanocellulose. In fact, the hydrophobic nature of the crystalline part of nanocellulose can be exploited to host hydrophobic molecules like Curcumin,[3] and this simple interaction can be obtained with a mechanochemical approach, such as ball milling. The other approach might be the classic covalent functionalization taking advantage of the on C6 of the glucose monomeric unit of the cellulose fiber. While the first approach suggests the production of an inhalation powder for the treatment of non-small cell lung cancer (NSCLC), the latter may be interesting for the development of bio-active surfaces for the treatment of breast and ovarian cancer, where Auranofin finds applicability.



commercially available sulphated
CrystallineNanoCellulose (CNC)

Figure 1: Example of covalent functionalization of nanocellulose.

[1] B. Thomas et al., *Chem. Soc. Rev.* **2018**, *118*, 11575-11625.
[2] S. Behzadi et al., *Chem. Soc. Rev.* **2017**, *46*, 4218-4244.
[3] T. S. Anirudhan et al., *Int. J Biol Macromol.* **2021**, *183*, 2044-2054.

POS05

Study of magnetic anisotropy of lanthanide complexes trough ab initio methodologies

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Lanthanide complexes are highly versatile molecular spin systems,[1] behaving as qubits for high-speed computation, or as Single Molecule Magnets for data storage. For quantum processing and molecular memory, recent studies reported that is possible to control the spin degrees of freedom via electric fields, which is easy to confine at sub-nanometric scale, environmentally friendly and fast to switch. In this context, the aim of my project is the computational investigation of the effects of applying electric fields on the magnetic properties of Ln(III)-complexes, a screening that would otherwise require expensive experimental techniques, with the goal of guiding the synthesis of optimized molecular systems for mentioned applications. My study will focus on non-centrosymmetric complexes with high axial symmetry, such as the series shown in figure,[2] which are expected to exhibit pronounced sensitivity to external fields and maximize the first-order spin-electric effect (the experimentally observable) due to the global asymmetry of the ligand field.

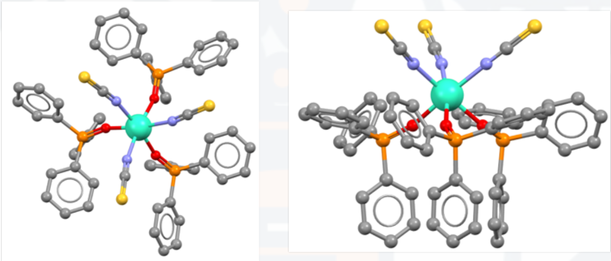

Figure SEQ Figure * ARABIC 1: [Ln($OPPh_3$)$_3$(NCS)$_3$] (Ln= any tripositive lanthanide ion) Left: along the C_3 axis. Right: view perpendicular to the C_3 axis. Colour code: Dy: aquamarine, N: blue, P: orange, O: red, C: grey. H omitted for clarity.

After the geometry optimization at DFT level in presence of an externally applied electric field, spin-Hamiltonian parameters will be computed using multiconfigurational wavefunction-based methods, which consider multiple electronic configurations and strong static correlation in open-shell lanthanide complexes. Preliminary calculations on [Dy($OPPh_3$)$_3$(NCS)$_3$] reveal significant axial magnetic anisotropy and a Kramers doublet distribution indicative of ground-state mixing with excited states. These properties, coupled with the sensitivity to local geometry, underscore their potential for quantum and magnetic applications.

[1] G. Aromí et al., *Handb. Phys. Chem. Rare Earths* **2019**, *56*, 1-54.
[2] S. A. Cotton et al., *Coord. Chem. Rev.* **2017**, *340*, 220-231.

POS06

Calcium Phosphate-Based Drug Delivery Nanosystems with Ionic Substitutions and Polymer Coatings for Applications in Nutraceuticals, Antitumor Therapies, and Bone Repair

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The development of advanced drug delivery systems is crucial to address the limitations of conventional therapies, such as poor bioavailability, low selectivity, and off-target effects. In this context, calcium phosphate (CaP)-based nanoplatforms represent a promising solution due to their biocompatibility, biodegradability, and chemical versatility.[1] This project focuses on the development of CaP-based nanosystems engineered with ionic substitutions, surface coatings and functionalizations or incorporation into hydrogel. The versatility of these systems enables their application across various field: in nutraceuticals delivery, in which protective coatings enhance stability and absorption of bioactive molecules in gastrointestinal tract;[2] in cancer therapy, where pH-sensitive CaP carriers enable selective release of anticancer drugs in acidic tumor environments;[1] in bone repair, in which CaP-based hydrogels act as injectable scaffolds, facilitating tissue regeneration.[1] To optimize the performances, key synthesis parameters (e.g. size and crystallinity) will be fine-tuned.

A Comprehensive characterization will be performed using techniques including Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Energy Dispersive X-ray Spectroscopy (EDX), Inductively Coupled Plasma Mass Spectrometry (ICP-MS), Thermogravimetric Analysis (TGA), CHNS elemental analysis, Fourier Transform Infrared Spectroscopy (FTIR), Confocal Raman Microscopy and X-ray Diffraction (XRD), to study morphology, composition and crystallinity. Particle size and surface charge will be assessed by Nanoparticle Tracking Analysis (NTA), Dynamic Light Scattering (DLS), and zeta potential measurements, while Gas adsorption porosimetry will evaluate the surface area. Drug release will be studied with UV-Vis Absorption Spectroscopy and High-Performance Liquid Chromatography (HPLC). Biological studies, including cytotoxicity, cellular uptake, and bone regeneration assays, will be carried out in collaboration with other research groups and will validate the efficacy and safety of the developed systems.

[1] T. J. Levingstone et al., *Nanomaterials*. **2019**, *9*, 145.
[2] A. A. Sable et al., *Pharmaceutics* **2024**, *16*, 423.

POS07

Immune-checkpoints response and Siglecs involvement as therapeutics targets.

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Immune checkpoints, such as CTLA-4, PD1, and PD-L1, act as regulatory mechanisms to prevent excessive immune activation and maintain self-tolerance. Their blockade using immune checkpoints inhibitors (ICIs) has emerged as a transformative strategy in cancer immunotherapy, reinvigorating T cell responses to eliminate tumors. However, despite their success, limitations such as immune-related adverse events (irAEs) and variable response rates highlight the need for novel targets to improve therapeutic outcomes.[1]

Siglecs (sialic acid-binding immunoglobulin-like lectins), a family of immunomodulatory receptors expressed primarily on immune cells, have gained attention as potential complementary targets in immunotherapy. These receptors modulate immune responses through the recognition of sialylated glycan structures, commonly exploited by tumor cells to evade immune surveillance. Siglecs, such as Siglec-7 and Siglec-9, suppress T cell and natural killer (NK) cell activity via ITIM-mediated inhibitory signaling. Targeting these pathways by disrupting Siglec-sialic acid interactions or by modulating downstream signaling, offers a promising strategy to enhance antitumor immunity.[2]

Combining ICIs with Siglec-targeting therapies may synergistically enhance immune activation while mitigating resistance mechanisms. Furthermore, Siglecs are implicated in maintaining immune homeostasis, presenting opportunities for addressing irAEs through selective modulation of these pathways. Ongoing studies are exploring the dual targeting of immune checkpoints and glyco-immunology to refine cancer treatments and expand applications to autoimmune and inflammatory diseases.[3]

[1] A. Hossain, Md. *Int. Immunopharmacol.* **2024**, *143*, 113365.
[2] H. Feng et al. *Cancers*, **2024**, *16*.
[3] A. Zhang et al. *Mol. Cancer* **2024**, *23* (1), 251.

POS08

Smart device for fish and seafood freshness and quality

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Fish and seafood are widely regarded as nutritious sources of protein, omega-3 fatty acids, and essential nutrients. However, they can accumulate contaminants from their environment or lose their freshness, posing potential risks to human health. Contaminants in seafood primarily include heavy metals (e.g., mercury, lead, and cadmium), persistent organic pollutants (such as PFAS, PCBs and dioxins), micro- and nanoplastics, and biotoxins produced by microbial pathogens. Biotoxins are probably the most concerning contaminants, since they can have severe effects on human health. The aim of this thesis will be the development of pocket device based on sensors and biosensors for on-site analysis of fish and seafood freshness and quality. Various approaches (including nanomaterials and biomimetic receptors) will be investigated for the sensors realization to achieve ultra-sensitive detection of contaminants, even in complex matrices.

POS09

Development and Characterization of Protein made Materials for Food Packaging Applications

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During a very long time and still as of today, plastics made from petrochemical polymers are a major part of our life, such as polyethylene, ethylene vinyl alcohol… a material that weighted more than 390 billion dollars in 2024 for the food packaging market.

To find an alternative to petroleum-based plastics is of vital importance in this day and age, and new solutions are rapidly emerging.

The use of polysaccharides and proteins are the two mains bio-alternatives to answer this problematic, and this thesis has for objective to use vegetal-based proteins to produce a novel material for food packaging: by the use of plasticizer, cross-linker and other additives, the goal is to design a film competitive enough with the petroleum-based materials.

The main characteristics to look at for a good film are: mechanical resistance, antioxidant activities, water vapor barrier, aspect, gas barrier, antibacterial properties and biodegradability.

The use a canola/rapeseed protein, a source of proteins that has yet to be extensively studied, would be our starting material for an efficient material as food packaging.

Figure 1: Life cycle of Biopolymer packaging material

[1] H. Chen et al., **2019**, *11*, *12*, 2039.
[2] B. Tajeddin et al., *Elsevier*, **2020**, 525-543.
[3] S. Aquilia et al., *Biomolecules*, **2024**, *14*, *8*, 982.

POS10

Sustainable Metal Deposition for Advancing High-Tech Materials

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The integration of metal deposition on polymeric substrates stands for a transformative approach that uses the lightweight, cost-efficient properties of polymers alongside the functional advantages of metals, easing the development of advanced high-tech devices.[1] This research investigates sustainable methods for polymer metallization, a critical advancement in achieving circular economy solutions across industries such as electronics, automotive, and fashion. The project emphasizes eco-friendly metallization processes,[2] avoiding the use of toxic reagents like chromium and formaldehyde, and employing techniques such as Electroless Deposition and Physical Vapor Deposition (PVD). These approaches enable the efficient production of thin, conductive metal films with improved durability and functional responsiveness. Recycled polymer substrates, including nylon, are prioritized to align with sustainability goals, and end-of-life disposal strategies are developed to meet the targets outlined in the European Green Deal. Key innovations include the development of tungsten- and iron-based alloys as sustainable alternatives to traditional lead-based X-ray shielding materials[3] enhancing safety in medical and industrial applications. Comprehensive material characterization using spectroscopic, diffractometric and microscopic techniques, including Scanning Electron Microscopy (SEM), X-ray Fluorescence (XRF), and X-ray Diffraction (XRD), ensures detailed evaluation of surface morphology and properties. Electrochemical studies further assess the efficiency of electroplating baths and confirm the performance of the resulting coatings. By upcycling waste textiles and plastics into high-performance materials, this project shows the potential of discarded resources in driving sustainable innovation. The recyclability of these metallized products promotes circular economic practices and minimizes waste. Additionally, their lightweight and high-performance characteristics contribute to energy efficiency in industrial applications.

[1] R. Melentiev, et al., *Materials & Design*, **2022**, *221*, 110958.
[2] W. Giurlani et al., *Sustainability*, **2024**, *16*, 5821.
[3] S. S. Belevskii et al., *SEAE*, **2020**, *56*, 1-12.

POS11

Energetic valorization of lignocellulosic biomasses from industrial manufacturing

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Beer manufacturing is characterized by a steady production of residues, such as brewery spent grains (BSGs), that represent the insoluble part of malted barley and the 85% of total brewing waste.[1] Globally, 36.4 million tons/year of BSGs are generated and later landfilled, releasing ~ 513 kg/ton of CO_2, or primarily recycled as low-value livestock fodder.[1] However, BSGs' shelf life is limited by its high moisture content (> 70%) and susceptibility to microbial spoilage.[1] Hydrothermal liquefaction (HTL) or carbonization (HTC) is a suitable thermochemical method to valorize low-quality wet lignocellulosic biomasses, without the need of any pre-drying step, to produce hydrochar and bio-oil, potentially applied as source of chemicals and biofuel intermediates.[2] The reaction exploits the water properties near and above its critical point (T_C = 374°C and P_C = 22 MPa), where it behaves as a non-polar solvent because the dielectric constant decreases by 80%, but the ionic product is high enough (above 10^{-14}) to favor ionic reactions.[2] *Rhodopseudomonas palustris* (*R. palustris*), a purple non sulfur bacterium (PNSB), has been applied in wastewater treatment to produce valuable compounds, such as hydrogen and biopolymers, via photofermentation.[3] The purpose of this project is to investigate the optimal conditions for the thermochemical treatment of BSGs via HTL or HTC and the microbial valorization with *R. palustris* of produced bio-oil and hydrochar.

[1] M. Jakowski et al., *Energies*. **2020**, *13*, 2058.
[2] B. Ciuffi et al., *Sci Rep*. **2021**, *11*, 15504.
[3] M. Li et al., *Front. Bioeng. Biotechnol*. **2022**, *10*.

POS12

Development of constructs for saccharide antigen's presentation

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Immunotherapy represents one of the most innovative procedures concerning tumor's treatment. Its aim is to stimulate the patience immunity system's own response against cancer cells, that usually escape normal control mechanisms.

Glycoconjugate architectures have proven to be a successful diagnostic method and also a good treatment option for many different tumors (such as pancreatic cancer, ovarian cancer, breast cancer). [1]

The aim of this project is to incorporate Tn, TF, STn and analogue antigens (associated to the MUC-1 family), into peptidic constructs, to have a multivalent system to modulate the immune system in a potent and persistent way. The selected platforms will be biocompatible and biodegradable, to be better administered and tolerated. [2]

The project will also include research on the use of peptidic platforms to present bacterial/viral antigens. In this case the target will be pathogen lectins, proteins that are responsible for mediating host cells binding infection.

[1] F. Corzana et al., *Angew. Chem. Int. Ed. Engl.* **2024**, (*e202407131*), 1521-3773.
[2] F. Papi et al., *Org. Biomol. Chem.* **2020**, *18 (37)*, 7366-7372.

POS13

Synthesis of Organic and Hybrid Organic-Inorganic Functional Materials for Heterogeneous Catalysis and Gas Storage

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Climate changes and their effects on the quality of life are the focus of public opinion; at the same time, scientific research is largely devoted to find solutions for decreasing the anthropogenic impact on the environment. The project focuses on the challenging topic of Carbon Capture and Utilization (CCU) for the valorization of the most abundant greenhouse gas: carbon dioxide (CO_2).

To this end, we propose the development of new synthetic strategies to the preparation of single-atom catalysts (SACs) based on light-weight heterodoped (i.e., N-doping) C-networks from the series of Covalent Triazine Frameworks (CTFs). Classically, this subclass of porous organic polymers is prepared from dicyanoaryl precursors *via* ionothermal conditions,[1] and exhibit high specific surface area, permanent micro/meso-porosity along with a prevalent amorphous nature. The presence of N-dopants is generally associated with an increase of the material surface electron density and basicity. While the former is thought to have a central role in the stabilization of metal SAs, the latter is claimed to facilitate the generation of local CO_2 concentration gradients[2] neighbouring to SAs that facilitate CO_2 reduction. Based on our previous works in the field,[3] we will investigate a novel protocol for the preparation of iron-based SACs, using an unconventional method for the generation of highly crystalline CTFs featured by well-dispersed iron SACs as active sites for the CO2RR reaction.

[1] G. Tuci et al., *Adv. Funct. Mater.*, **2017**, *27*, 1605672.
[2] M. Moro et al., *ACS Materials Lett.*, **2024**, *6*, 583-589.
[3] X. Zhang et al., *J. Mater. Chem. A.*, **2022**, *10*, 6153.

POS14

Development of a new strategy for the inhibition of chemical and biological degradation on black-and-white photographs

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This project focuses on developing a novel and multidisciplinary approach to monitor, inhibit, and prevent the chemical and biological degradation of black-and-white (B&W) ancient photographs mainly focusing the attention on the photographic emulsion. Photographic materials (i.e. photographs and negatives) are multi-layer objects made of various types of supports: an emulsion composed of micrometric silver clusters and a binder (typically gelatin, albumin, or collodion), and a protective varnish. The degradation of the photographic emulsion can be caused by microbial activity, light exposure, and high humidity and temperature, affecting both the silver and the binder. Thus, the conservative strategy imposes the storage of photographs in a dark and ventilated environment at controlled and low RH and temperature (T ≈ 4°C and RH ≈ 30-50%), with enormous maintenance costs.[1] The most common solution to stop biological contamination is the application of synthetic biocides, which are toxic and potentially have a high environmental and health impact. In this context, developing novel "green" systems to inhibit both biological and chemical degradation is mandatory. The first step of this project will concern the non-invasive characterisation of the photographic materials and their degradation products using optical techniques (e.g. Optical Coherent Tomography-OCT and Reflectance Imaging Spectroscopy-RIS). Microorganisms present in photographs will be identified through culture-based methods and metagenomics techniques. Then, the attention will be focused on the development of "green" systems that will act as both antimicrobial agents and inhibitors of the acid hydrolysis of the binder, such as nanocellulose-based gels. These systems will be loaded with nanoparticles[2] (e.g. TiO_2, $Ca(OH)_2$, and $CaCO_3$ NPs) and essential oils with biocidal properties.[3] Moreover, the effectiveness of these charged gels in inhibiting decay will be evaluated in the case of both direct application onto the photographic surface and by placing them in the same closed environment to act as inhibitors of further contaminations.

[1] L. Bertrand, *Getty Conservation Institute*, *Los Angeles*, **2003**, *285*.
[2] M. E. David et al., *Materials* **2020**, *13*, 2064.
[3] A. P. Santo et al., *Sci. Total Environ,* **2023**, *877*, 162913.

POS15

Covalent Podands and Macrocycles for the Molecular Recognition of Carbohydrates

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Carbohydrates are the most versatile tools in nature.[1] In fact, they are the most abundant molecules in biology. Carbohydrate-protein molecular recognition plays a vital role in several physiological and pathological processes, and there is a growing need for new chemical tools for the molecular recognition of carbohydrates.[2] However, saccharides are rather difficult ligands to recognise in water.[3] Nonetheless, several efforts have been made in the long run and synthetic receptors effective in water have been recently appeared in the literature. Here we propose to synthesise macrocyclic and acyclic synthetic receptors by varying the different building blocks that fulfil complementarity for efficient binding and high selectivity. This will include aromatic groups for CH-π interactions with the aliphatic backbone of the carbohydrate, hydrogen bonding groups to interact with the polar groups of the sugar and hydrosolubilising groups to ensure water solubility. We would also like to further exploit this by immobilising the receptors on a solid support, thereby developing functionalities including separation of carbohydrate (containing) molecules, sensors for biologically relevant saccharides, and drug delivery systems that actively target carbohydrates.

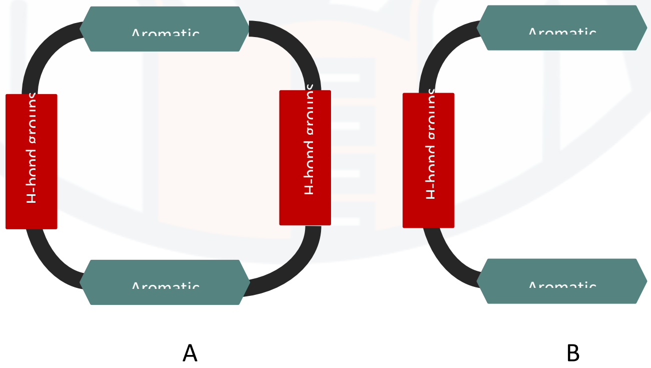

Figure 1: Schematic representation of synthetic receptors A) Macrocycle B) Acyclic.

[1] A. Varki, *Glycobiology*, **2017**, *27*, 3-49.
[2] O. Francesconi et al., *ChemBioChem*, **2019**, *20*, 1329-1346.
[3] F. Milanesi et al., *Chempluschem*, **2024**, *89*, e202300598.

POS16

Innovative approaches for sustainable metal coating for energy applications and the Made in Italy industry

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The global demand for high-quality metal coatings from the electroplating industry, essential for global manufacturing processes across energy, electronics, automotive, and fashion sectors, faces the critical challenge of metal scarcity. The shortage of strategic metals calls for striving toward optimized electrodeposition processes and advanced physical vapor deposition (PVD) techniques. Key objectives of this project include not only improving metal usage efficiency but also focusing on the recovery and reintegration of metals into the circular economy, specifically in the hydrogen-based field as electrocatalysts.

Multiphysics simulations are employed to optimize current density distribution during electrodeposition, which minimizes metal waste and ensures uniform coating thickness. Integrating theoretical models with experimental data provides a comprehensive approach to advancing metal coating technologies while supporting global sustainability initiatives.[1] Further advancements in PVD are explored to eliminate the need for electrochemical pretreatments, thus reducing reliance on traditional electroplating methods.[2] Additionally, the project addresses environmental concerns by developing strategies for recovering metals from industrial wastewater, and upcycling these recovered materials into valuable electrocatalysts for energy applications, such as Pd(II)-based catalysts for oxygen reduction reaction (ORR).[3]

This research includes morphological, compositional and structural characterization by microscopic and spectroscopic methods of the metal deposits and electrocatalysts obtained. Corrosion tests are performed to characterize PVD-coated artifacts. Finally, electrochemical characterization is carried out to test the electrocatalyst efficiency using a rotating ring-disk electrode (RRDE).

Expected outcomes encompass improved process efficiencies, reduced environmental impact, and the promotion of sustainable practices within the electroplating industry, supporting global sustainability initiatives aligned with the United Nations Agenda 2030.

[1] W. Giurlani et al., *Sustainability*. **2024**, *16*, 5821.
[2] M. Vorobyova et al., *Materials*, **2023**, *16*, 4919.
[3] M. Bonechi et al., *Catalyst*, **2021**, *11*, 764.

POS17

Stereocontrolled synthesis of polyhydroxylated iminosugars: from small molecules to polymer decoration for antibacterial applications

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Iminosugars, glycomimetics belonging to the class of polyhydroxylated alkaloid family, emerged over the years as promising therapeutic agents due to their ability to interfere with biological processes involving carbohydrate processing enzymes. While iminosugar-based drugs are currently on the market or under clinical trials for treating a wide range of diseases (e.g. diabetes, lysosomal storage disorders, viral infections, etc..), their potential as antibacterial agents was poorly investigated. To fill this gap, a general versatile strategy which employs an enantiomerically pure cyclic nitrone easily obtainable from biomass-derived sugar D-arabinose and a totally selective cycloaddition allows to fully regulate the absolute stereochemistry of the many stereogenic centres that adorn these compounds. Using *N,N*-dimethylacrylamide as dipolarophile, the strategy lead to easily synthesize 7-deoxycasuarine derivatives[1] with OH, -NH_2 or -N_3 groups at carbon C-6 that can be coupled with long alkyl chains through different functional groups (esters, carbamate, amide, urea, triazole etc.). Using a BCN (bicyclo[6.1.0]non-4-yne) derivative as dipolarophile, a series of new polyhydroxylated pyrrolidines will be accessible via SPANC (strain-promoted alkyne-nitrone cycloaddition) reactions[2] using bioorthogonal and green conditions. The antibacterial properties of all the new compounds will be investigated, determining their MIC (Minimum Inhibitory Concentration) against various bacterial strains. The most promising candidates will be used for further functionalization with chitosan biopolymer due to its well-known antibacterial activity (Figure 1), looking for a synergistic effect.

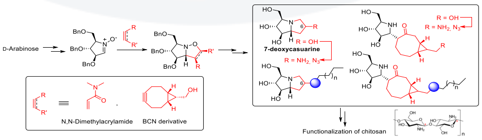

Figure 1: Synthesis of small molecules and conjugation with polymers.

[1] A. Brandi et al., *Chem. Eur. J.* **2009**, *15*, 7808-7821.
[2] A. Bilodeau et al., *Chem. Rev.* **2021**, *121*, 6699-6717.

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POS18

Implementation of a database of contaminants of emerging concern as training set of preconcentration protocols for non-target analysis

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The ever-increasing production and use of chemicals worldwide represent a real threat, with obvious consequences on the quality of the acquatic ecosystem services provided, such as raw water to be treated for drinking purposes or to be used for the irrigation of edible crops.[1] To monitor chemical contaminants of emerging concern (CECs) and their transformation products (CEC-TPs), non-targeted analysis (NTA) platforms based on liquid chromatography (LC) coupled with high-resolution mass spectrometry (HRMS) is the techniques of choice to respond to the urgent need of comprehensive qualitative data on the chemical health status of aquatic ecosystems.[2,3] NTA, although performed through virtually comprehensive instrumental analytical platforms, is limited in practice, in fact insufficient retention of certain peaks and their consequent broadening, result in challenging issues in the acquisition of MS2 spectra, which are necessary for the identification of unknown features. Poor sensitivity of non-target analytical platforms is another problem, which limits their virtually comprehensive attribute. To address these problems, extraction systems for preconcentrating a wide range of analytes prior to non-target analysis are required. These pre-concentration methods must be tested on appropriate training sets that guarantee a high chemical coverage. Many databases available that could be used for this purpose have limitations such as the lack of transformation products, which make them only partially usable in non-target analyses of environmental matrices. Based on these considerations, a database containing representative CECs from various environmental scenarios has been implemented, including precursors, metabolites, transformation products, and isomers. To implement such a database, the current European regulations and Watchlists, CECs reported in literature as pollution markers of relevant water bodies, and TPs predicted in silico by software are considered.

[1] Y. Du et al., *Sci. Total Environ.* **2022**, *806*, 150691.
[2] M. Paszkiewicz et al., *Trends Analyt. Chem.* **2022**, *154*, 116671.
[3] A. Müller et al., *Chemosphere*, **2011**, *85*, 1211-1219.

POS19

Complexes on a bookshelf: A library for a better understanding of Spin-Electric effects

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One of the most promising fields in developing new technologies is the one of quantum technologies and molecular magnetism. One of the newest discoveries is the exploitation of an electric field to address magnetic properties. This interaction at a molecular level is called Spin-Electric effect. This subject is poorly explored and the few works related to molecules focus on metal cluster or chains.[1] The main problem behind SE effects is that its experimental detection is very hard and for now is only related to EPR techniques. The magnitude of SE effects is much smaller than magnetic effects so for now we need to relay to the high sensitivity of the EPR and that limits the study to system that are EPR active.[2]

This Doctoral Project aims to exploiting chemistry and molecular magnetism to find suitable candidates to experimentally investigate SE effects and to define how we can tailor the structure of a molecule to control its functionality. During my Master Thesis I have carried out a complete magnetic characterization of an isostructural series of three Cobalt (II) complexes. The three complexes of CoX_2-NNN are described by a strongly anisotropic *g-factor* and a rhombic ZFS with a high and negative D that decreases, in absolute value, along the series. All the three systems give crystals with an acentric unit cell and if diluted with a Zn-based diamagnetic analogue are EPR active, making these systems candidates to the study of Spin Electric effects. I choose Cobalt as metal ion because it has tuneable magnetic properties thanks to the presence of non-quenched orbital angular momentum.[3] This tuneability suggests the possibility of using Cobalt complexes in order to create a library of complexes with known SE effect. The perfect way to do so is exploring the possible functionalization of the Cobalt (II) isostructural series. The halide-Co bond is very reactive and that suggest the possibility to functionalize the complex by substitution of the halide with different donor ligand. Another possibility is to study long range effect with the functionalization of benzene ring of the pincer ligand NNN.

[1] A. Kiel et al., *Phys. Rev. B*, **1972**, *5*, 803-813.
[2] M. Fittipaldi et al., *Nat. Mater.* **2019**, *18*, 329-334.
[3] O. Kahn, *Molecular Magnetism*, **1993**.

POS20

Development of natural encapsulation systems for the controlled release of active molecules

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This research explores the development of natural encapsulation systems for controlled release of active molecules, addressing the growing demand for sustainable and environmentally friendly technologies in sectors such as cosmetics, nutraceuticals, agrochemicals, and medicine. Key materials include zein, the main storage protein in corn, recognized as GRAS compound by the FDA,[1] and keratin, one of the most abundant structural proteins present in mammalian hair, such as wool and human hair. While wool is widely utilized in the textile industry, human hair is often regarded as waste and typically discarded, and this contributes significantly to annual pollution levels.[2] Developing keratin-based materials could offer a sustainable strategy to address this issue, transforming an underutilized resource into valuable applications.

Active molecules, predominantly hydrophobic and/or volatile, will be encapsulated via the formation of core-shell capsules starting from a Pickering emulsion as template or directly, leveraging the amphiphilic properties of the selected proteins and suggesting a possible green alternative to surfactants as emulsion stabilizers. Our focus will be on tailoring the conformational and functional properties of proteins for the formation of homogeneous and robust coatings imparting stability and functionality enhancement to the final delivery systems.[3] This approach ensures effective dispersion in the final environment, both polar and apolar, depending on the specific interaction of the active molecule and the protein.

A plethora of characterization techniques such as: Dynamic Light Scattering (DLS), Zeta potential, Scanning Electron Microscopy (SEM), Differential Scanning Calorimetry (DSC), Thermogravimetric analysis (TGA), UV-Visible spectrophotometry, Dynamic Head Space (DHS) and Gas Chromatography-Mass Spectroscopy (GC-MS), will be applied to assess the stability, encapsulation efficiency and release kinetics over time and under different conditions.

[1] C. Sun. et al. *Food Hydrocolloids*, **2016**, *58*, 11.
[2] C. Ferroni et al. *Appl. Sci.* **2021**, *11*, 9417.
[3] M. Pascoli et al. *Front. Chem.* ***2018**, 6*, 6.

POS21

Machine Learning-Assisted Imprinting Analysis of Epitopes in Polynorepinephrine Biopolymers via (L)SPR Assay

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The dream of having innovative materials capable of functioning as affinity "binding partners" instead of antibodies is a groundbreaking research field in bioanalytics and biosensing, aligned with EU directive on *animal protection in research* (2010/63/EU). Molecularly Imprinted Polynorepinephrine (MIPNE), synthesized by co-polymerizing Norepinephrine (NE) with a peptide following the "Epitope Imprinting Approach" (EIA), constitutes a promising alternative.[1] EIA improves receptor performance by selecting and imprinting a specific peptide sequence from a target protein,[2] rather than the whole protein itself. A key challenge, however, remains in defining optimal selection criteria for epitopes, which significantly impacts the sensitivity and stability of the receptor and, consequently, the biosensor's performance.

Here is introduced an innovative, Machine Learning-assisted method for epitope selection. Developed starting from an LSPR assay, this method overcomes the unreliability of the traditional "trial and error" approach. A training library of 50 peptides was analyzed by measuring the maximum plasmonic absorption wavelength of AuNPs grown directly on each MIPNE.[3] Results clustered into distinct output classes, used as experimental labels. From this data, 101 peptide descriptors from Python environment were extracted and correlated with the experimental classes, leading to reliable descriptors capable of predicting optimal peptide templates based on the protein's sequence. The method was finally validated through affinity and kinetic SPR assays, confirming its effectiveness.

[1] F. Torrini et al., *Sens. Actuators B Chem.* **2023**, *383*, 133586.
[2] F. Torrini et al., *Biosens. Bioelectron.* **2022**, *217*, 114706.
[3] S. Scarano et al., *Microchimica Acta*, **2019**, *186*, 1-7.

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POS22

Design, synthesis and biological evaluation of SARS-CoV-2 peptides: diagnostic and therapeutic applications

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Since pandemia, the SARS-CoV-2 virus has attracted significant research interest. Among the numerous areas of investigation, one of the most extensively studied is the mechanism by which the virus interacts with human cells to trigger viral replication. Fundamental to this process is the Spike protein, a glycoprotein on the surface of the virus lipid envelope, which plays a pivotal role in mediating viral entry into host cells.[1] Due to the critical role of this protein in the infection process, it serves as both an immunological and therapeutic target. This project aims to develop peptides derived from the Spike protein to pursue two primary aims: first, to study the immune response of vaccinated patients with varying clinical backgrounds, and second, to design novel and effective antiviral therapies against SARS-CoV-2. For the first aim, immunological studies will evaluate both the duration and efficacy of the immune response elicited by vaccination in healthy individuals and those with pre-existing conditions. For the second aim, antiviral peptides mimicking sequences of the Spike protein will be synthesized to disrupt the protein-protein interactions critical to viral infection.[2] The peptides will be synthesized using solid-phase strategies (SPPS) with both microwave and induction-heating automated synthesizers. Their conformations will be analyzed through circular dichroism and nuclear magnetic resonance spectroscopy to perform structure-activity relationship studies. Finally, immunological assays and *in-vitro* tests, to evaluate antimicrobial activity, will be carried out.[3]

[1] D. Wrapp et al., *Science*, **2020**, *367*, 1260-1263.
[2] M. A. Stincarelli et al., *Virus Research*, **2023**, *334*, 199170.
[3] M. Quagliata et al., *ACS Omega*, **2023**, *8*, *25*, 22665-22672.

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Conjugation strategies toward the development of carbohydrate-based vaccines against *Acinetobacter baumannii*

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Acinetobacter baumannii is a gram-negative, opportunistic pathogen frequently associated with hospital-acquired infections, particularly in immunocompromised patients. Its multidrug resistance and persistence in healthcare environments pose a significant global health threat, underscoring the urgent need for effective vaccine strategies.[1]

As part of the MSCA-funded ACINETWORK PhD program, my research aims to identify novel approaches for developing glycoconjugate vaccines against *A. baumannii*. This strategy leverages immunogenic carriers, such as proteins, to enhance the immunogenicity of saccharide antigens, eliciting robust and long-lasting immune responses.[2] My project focuses on optimizing chemical conjugation protocols to develop a modular, scalable, and efficient methodology for linking saccharide antigens to carriers. Additionally, nanoparticles are explored as innovative multivalent platforms to conjugate diverse oligosaccharide antigens, either targeting a single *A. baumannii* strain or combining antigens from multiple strains.

These glycoconjugates will aid to the identification of the minimal binding epitopes recognized by anti-*A. baumannii* antibodies, providing critical insights for designing next-generation vaccines against this multidrug-resistant pathogen.

[1] F. Perez et al., *Antimicrob. Agents Chemother.*, **2007**, *51*, 3471-3484.
[2] R. Adamo, *Acc. Chem. Res.*, **2017**, *50, 5*, 1270-1279.

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