BOOK OF ABSTRACTS

12th FRENCH-ITALIAN CHEMISTRY DAYS

Welcome

Dear Participants, Dear Colleagues, Dear students,

We would like to thank you for your kind participation to the XII edition of the French-Italian Chemistry Days (Giornate Italo-Francesi della Chimica, GIFC 2026), organized by the Provence-Alpes-Côte d'Azur section of the Société Chimique de France (SCF) and the Piemonte/Valle d'Aosta and Liguria Sections of the Società Chimica Italiana (SCI). This 2026 edition is organized in Nice and we are very grateful to the Université Côte d'Azur for hosting us. We also warmly thank all our academic and industrial sponsors for their generous support.

This event is organized every two years alternately in the two countries: in 2002 in Juan-les-Pins, in 2004 in Genoa, in 2006 in Turin, in 2008 in Nice, in 2010 in Genoa, in 2012 in Marseille, and in 2014 in Turin, 2016 in Avignon, 2018 in Genoa, 2022 in Toulon and 2024 in Turin. The French-Italian Chemistry Days therefore represent a dynamic platform for interdisciplinary collaboration, fostering lasting connections among researchers in the Provence-Alpes-Côte d'Azur region and those in the Piemonte/Valle d'Aosta and Liguria, under the auspices of either SCF or SCI. This event also aims to facilitate enhanced scientific and cultural interaction at the European level.

The scientific program will be enriched by plenary lectures delivered by internationally renowned experts, alongside oral and poster presentations by early-career researchers (PhD students and postdoctoral fellows) selected for their excellence by the Scientific Committee. In total, the two-day program will feature 4 plenary lectures, including the 2 distinguished awards recognizing outstanding contributions from a French and an Italian chemist, 5 invited talks, and 36 oral communications. Special emphasis will be placed on supporting the next generation of scientists: poster sessions and oral contributions will be driven by young chemists, and 3 presentations will honor the 2026 Thesis Prizes, awarded by the South-PACA section of the French Chemical Society (SCF) and the regional sections of Piemonte – Valley d'Aosta and Liguria of the Società Chimica Italiana (SCI).

Your participation to this event not only contributed to its success but also aligned your research with cutting-edge developments in various chemical areas, including organic and bioorganic chemistry, green chemistry, material chemistry, computational chemistry and AI, and medicinal and food chemistry.

We hope that this congress will provide an excellent platform to showcase both advancement and innovation within the chemical sciences and that it will be a great opportunity for all researchers, especially the PhD students who can live a truly educating and enriching experience, including prominent visibility throughout the event, and the opportunity to engage with leading researchers and professionals in the field.

The 2026 XII edition of the French-Italian Chemistry Days organizing committee

Schedule

April 9th 2026

8h00-8h20	Welcome of participants		
8h20-8h30	OPENING ADDRESSES: Dr. Sylvain Antoniotti (UniCA IDEX Vice-President) (Dr. Y. Coquerel, Prof. V. Michelet)		
	Moderators: Andrea Basso & Yoann Coquerel		
8h30-9h10	PL	Pr. Orietta Monticelli (ITALY)	
9h10-9h50	PL	Pr. Laurence Charles (FRANCE) (Winner of the Grand Prix SCF-Sud-PACA)	
9h50-10h00		Career Achievement Award: Pr. Giorgio Cevasco (ITALY)	
10h00-10h40	COFFEE BREAK		
	Parallel sessions		
		Valrose theater	Chemistry Amphitheater
		Moderators: Andrea Basso & Gaëlle Chouraqui	Moderators: Yoann Coquerel & Maela Manzoli
10h45-11h00	COM	CO1 JORANDON Mathieu	CO7 GUERRUCCI Sara
11h00-11h15	COM	CO2 GORRETA Giulia	CO8 KANDI Suryaprakash
11h15-11h30	COM	CO3 VIGROUX Alban	CO9 GIANOGLIO Luca
11h30-11h45	COM	CO4 RABONI Francesco	CO10 VASHCHENKO Oleksii
11h45-12h00	COM	CO5 BAUBIAT Emma	CO11 CASALE Michael
12h00-12h15	COM	CO6 VIGO Christian	CO12 CHEBAIKI Mélina
12h15-13h15	LUNCH BUFFET		
	Moderators Maela Manzoli & Véronique Michelet		
13h15-13h45	IL	Dr. Olivier Chuzel (FRANCE)	
13h45-14h15	IL	Pr. Barbara Bonelli (ITALY)	
14h15-14h45	IL	Dr. Jean-Guy Boiteau (Industrial Invited lecture, FRANCE)	
14h45-14h50		Flash Communications Advion / Fluorochem / ICN Platform	
14h55-15h40	COFFEE BREAK		
	Parallel sessions		
		Valrose Theater	Chemistry Amphitheater
		Moderators: Maela Manzoli & Philippe Marsal	Moderators: Hervé Clavier & Francesca Spyrakis
15h45-16h00	COM	CO13 LY Minh Tu	CO19 NOVA Niccolò
16h00-16h15	COM	CO14 CANO Flavia	CO20 VITALE Benedetta
16h15-16h30	COM	CO15 SICCARDI Marion	CO21 AIT MOULAY Khadija
16h30-16h45	COM	CO16 DI GIORGIO Emmanuela	CO22 TREVIA Riccardo
16h45-17h00	COM	CO17 TRAPP Mathilde	CO23 BELKESSA Nawel
17h00-17h15	COM	CO18 VENTURI Sara	CO24 GAMBETTA VIANNA Julia
17h15-18h45	GET TOGETHER – POSTER SESSION		

Gala Dinner (20h-23h00)

April 10th 2026

8h00-8h30	Welcome of participants		
	Moderators Maela Manzoli & Yoann Coquerel		
8h30-9h10	PL	Dr. Raphaël Rodriguez (FRANCE)	
9h10-9h50	PL	Pr. Francesca Spyrakis (ITALY)	
9h50-10h30	COFFEE BREAK		
	Parallel sessions		
		Valrose Theater	Chemistry Amphitheater
		Moderators: Andrea Basso & Jade Dussart-Gautheret	Moderators: Romain Melot & Francesca Spyrakis
10h30-10h45	COM	CO25 RICCI Marco	CO31 VILLARD Gustave
10h45-11h00	COM	CO26 GUEDU Eden	CO32 WANG Zhen
11h00-11h15	COM	CO27 ANDREANA Ilaria	CO33 NICOLAS Jean
11h15-11h30	COM	CO28 GANDLEVSKIY Nikita	CO34 ANDINO Manuel
11h30-11h45	COM	CO29 GRASSO Federica	CO35 MAAREK Elsa
11h45-12h00	COM	COM 30 ALLAHI Shahin	CO36 CLARIN Mathilde
12h00-13h15	LUNCH BUFFET		
	Moderators: Andrea Basso & Kristina Plevova		
13h15-13h45	IL	Pr. Élise Dumont (FRANCE)	
13h45-14h15	IL	Dr. Matteo Lusardi (ITALY)	
		Moderators: Andrea Basso & Hervé Clavier & Maela Manzoli	
14h15-14h30	COM	Dr. Giulia Pellis, ITALY	
14h30-14h45	COM	Dr. Blanche Krieguer, FRANCE	
14h45-15h00	COM	Dr. Edoardo Donadoni, ITALY	
15h00-15h15	CLOSING REMARKS – POSTER & ORAL COM AWARDS		

Scientific Committee

The **Scientific Committee** is composed of the members of the SCF PACA, Liguria and Piemonte – Valley d'Aosta sections and of the local organizing committee.

Andrea Basso (University of Genova)

Gaëlle Chouraqui (Aix-Marseille University)

Hervé Clavier (Aix-Marseille University)

Yoann Coquerel (Aix-Marseille University)

Jade Dussart-Gautheret (Université Côte d'Azur)

Anthony Kermagoret (Aix-Marseille University)

Maela Manzoli (University of Turin)

Philippe Marsal (Aix-Marseille University)

Romain Melot (Université Côte d'Azur)

Véronique Michelet (Université Côte d'Azur)

Paolo Oliveri (University of Genova)

Kristina Plevova (Université Côte d'Azur)

Francesca Spyrakis (Università degli Studi di Torino)

Local Organizing Committee

Jade Dussart-Gautheret

Romain Melot

Véronique Michelet

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ICR
Institut Chimie Radicalaire


iSm2


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Le réseau des chimistes
DCO
Division de Chimie Organique


I C N
Institut de
Chimie de Nice

Awards

During the congress, the scientific commity will select **4 best oral communications** and **4 best research poster awards**.

We have also one extra award for the best research poster selected by you. So please, don't forget to vote by using QR code.

Best oral communication award

Best research poster award

Plan of the campus

The 12th edition of the French-Italian Chemistry Days (JFIC) will take place at the Théâtre du Grand Château and Amphi Chimie located in Valrose Campus of Université Côte d`Azur.

Address: 28 Avenue Valrose, Nice Cedex 2 06108, France

How to Reach Us:

- **By tram:** Take Line 1 (Tram T1) to the Valrose Université station.
- **By Bus:** Lines 11 and 37 also to the Valrose Université station.

Once on tram and bus stop *"Valrose Université"* and then please follow the picture below to reach the Théâtre du Grand Château (red cycle) or Amphi Chimie (blue cycle).

PLENARY LECTURES

Chemistry area :

□ Organic and Bioorganic Chemistry
X Green Chemistry
□ Material Chemistry
□ Computational Chemistry and AI
□ Medicinal and Food Chemistry

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Université Côte d'Azur
April 9th-10th 2026

PL-1

Bioplastics: the future of polymer materials?

Damonte, G.; Pellis, A.; Cozzani M.; Fortunato A.; Giribaldi L.; **Monticelli O.**

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Dipartimento di Chimica e Chimica Industriale, Università di Genova, Via Dodecaneso 31, 16146 Genova, Italy

Currently, the European Union is actively promoting the transition to a circular economy by implementing policies that encourage the development of sustainable products, services, and business models. The aim is to create an economic system based on the efficient use of natural resources and the reduction of waste and pollution. In this context, several urgent challenges related to plastic production, use, and pollution have been identified, including single-use items, excessive packaging, littering, microplastic release, high carbon footprints, and inadequate labelling systems. To address these issues, strategic actions focus on supporting the bio-based industry and establishing a comprehensive regulatory framework for bio-based, biodegradable, and compostable plastics. These materials, known as "bioplastics", whether bio-based, biodegradable, or both, have been the subject of extensive global research and debate. Despite their potential, several challenges remain regarding their production and application. These include high production costs, lower performance compared to conventional plastics, possible feedstock competition with the biofuel and food industries, risks in mechanical recycling streams, lack of dedicated composting and recycling infrastructure and logistics, and uncertainty regarding durability and biodegradability in different open environments.

In this scenario, this presentation begins with an analysis of the evolution of polymer materials towards bioplastics, highlighting research aimed at improving their properties through chemical modifications[2], polymer blending[3], and the incorporation of functional additives, as well as studies on their end-of-life[4-6]. Regarding this latter aspect, novel chemical recycling approaches are presented, based on the use of compounds from renewable sources and methods that are easily scalable and environmentally friendly, allowing the production of both linear and branched oligomers with different functionalities for application in various fields.

[1] European Commission. The European Green Deal COM (2019) 640 Final; European Commission: Brussels, Belgium, 2019.
[2] G. Damonte, F. Cantamessa, A. Fina, O. Monticelli, *Reactive and Functional Polymers*, 2023, 184, 105515.
[3] G. Damonte, R. Spotorno, D. Di Fonzo, O. Monticelli, *ACS Applied Polymer Materials*, 2022, 4, 6521.
[4] G. Damonte, L. Dullaert, A. Pellis, L. Giribaldi, O. Monticelli, *European Polymer Journal*, 2026, 246, 114563.
[5] G. Damonte, M. Cozzani, M. Ozenda, C. Siracusa, M.J. Calandri, A. Pellis, G.M. Guebitz, O. Monticelli, *International Journal of Biological Macromolecules*, 2025, 319, 145457.
[6] G. Damonte, A. Vallin, L. Giribaldi, A. Pellis, M. Hakkarainen, S. Subramaniyan, O. Monticelli, *Sustainable Materials and Technologies*, 2025, 43, e013

Chemistry area :

□ Organic and Bioorganic Chemistry
□ Green Chemistry
X Material Chemistry
□ Computational Chemistry and AI
□ Medicinal and Food Chemistry

12th French-Italian Chemistry Days
Université Côte d'Azur
April 9th-10th 2026

PL-2

Tandem Mass Spectrometry of Digital Polymers: from Design to Sequencing

Laurence Charles

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Aix Marseille University-CNRS, Institute for Radical Chemistry, Marseille, France

In the last decade, massive and long-term data storage in synthetic polymers has been proposed as an alternative to currently employed hard disks that require energy-consuming data centers to store quintillion bytes of data generated every day. Using modern polymer synthesis, a binary code can indeed be implemented in sequence-defined chains using two interchangeable monomers defined as 0-bit and 1-bit, respectively. As long as the two monomers have different mass, tandem mass spectrometry (MS/MS) is the most efficient sequencing method to "read" information "written" in such digital polymers. However, MS/MS sequencing is limited to quite short chains that are not suitable to massive data storage. To address this issue, the structure of digital polymers can be specifically tailored to control their dissociation behavior and hence achieve error-free reading of long chains. This MS/MS-assisted strategy is best illustrated by the case of poly(phosphodiester)s (PPDEs): careful optimization of each building block and polymer architecture permits to manipulate the charge state, the number and stability of fragments as well as storage density of monomers. Accordingly, high-capacity PPDEs containing hundreds of bits per chains can now be synthesized and efficiently sequenced using a routine mass spectrometer.

Chemistry area :

X Organic and Bioorganic Chemistry
□ Green Chemistry
□ Material Chemistry
□ Computational Chemistry and AI
□ Medicinal and Food Chemistry

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PL-3

Chemical Control of Cell Adaptation

Rodriguez, R.*; Müller, S.; Caneque, T.

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Cells can adopt distinct states independently of genetic alterations, a biological process commonly referred to as 'cell-state transition'. Acquisition of distinct cell states is characterized by the upregulation of the plasma membrane glycoprotein CD44 in development, immunity and cancer. Although often described as a cell-surface marker, the molecular function of CD44 has remained elusive for half-a-century. We found that CD44 mediates the uptake of specific metals, including copper and iron using hyaluronate carriers in various tissue types. This glycan-mediated metal endocytosis mechanism enables immune cell activation and acquisition of a drug-tolerant state of cancer cells (cell adaptation). Increase of copper(II) in mitochondria sustains NAD(H) redox cycling, promoting the production of metabolites that co-regulate the epigenetic programming of cell identity. In contrast, increase of iron in the cell nucleus fuels the activity of specific iron- and ketoglutarate-dependent demethylases, enabling specific transcriptional programs. We developed new classes of small molecules that selectively interfere with these metal-catalyzed chemical processes in cells. Inactivating mitochondrial copper(II) prevents acute inflammation in vivo demonstrating that control of cell-state transition confers therapeutic benefits. Pharmacological activation of lysosomal iron, on the other hand, induces ferroptosis in drug-tolerant persister cancer cells, impacting tumor progression. These findings illuminate a universal metal ion uptake mechanism and the critical role of metal ions as regulators of cell adaptation, paving the way towards the development of next generation therapeutics.

Activation of lysosomal iron triggers ferroptosis in cancer. T. Cañeque,…, R. Rodriguez*. ***Nature*** 642, 492-500 (2025).
Ageing of stem cells reduces their capacity to form tumours. T. Cañeque, R. Rodriguez* ***Nature*** 637, 36-37 (2025)
Multiple estradiol functions inhibit ferroptosis and acute kidney injury. W. Tonnus,…, R. Rodriguez,…, A. Linkermann*. ***Nature*** (10.1038/s41586-025-09389-x)
Lymph node environment drives FSP1 targetability in metastasizing melanoma. M. Palma,…, R. Rodriguez,…, J. M. Ubellacker*. ***Nature*** (Accepted for publications)
A druggable copper-signalling pathway that drives inflammation. S. Solier,…, R. Rodriguez*. ***Nature*** 617, 386-394 (2023).
Copper catalyses changes in cell state. S. Müller, R. Rodriguez*. ***Nature*** (10.1038/d41586-023-01330-4)
Chemical inhibition of NAT10 corrects defects of laminopathic cells. D. Larrieu,…, R. Rodriguez*, S. P. Jackson*. ***Science*** 344, 527-532 (2014)

Chemistry area :

□ Organic and Bioorganic Chemistry
□ Green Chemistry
X Material Chemistry
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□ Medicinal and Food Chemistry

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PL-4

Computational Multiscale Strategies to Interfere with NLRP3 Inflammasome Formation and Activation

Francesca Spyrakis [1]; Riccardo Scoccia [1]; Eleonora Gianquinto [1]; Elisabetta Marini; Massimo Bertinaria [1]; Giorgio Colombo [2]

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(1) Department of Drug Science and Technology, University of Turin, Italy

(2) Department of Chemistry, University of Pavia, Italy

The NLRP3 inflammasome is a cytosolic signal-recognition complex that integrates diverse perturbations of cellular homeostasis into inflammatory output. Following transcriptional priming and a second activation step triggered by additional inflammatory signals (e.g., ionic fluxes, lysosomal injury, and mitochondrial dysfunction), NLRP3 oligomerizes with ASC and pro–caspase-1 to drive IL-1β/IL-18 maturation and gasdermin D–dependent pyroptosis. Dysregulated NLRP3 signalling has been linked to a broad spectrum of inflammatory and neurodegenerative disorders, establishing NLRP3 as a high-value target for the development of new therapeutics.

We applied all-atom and coarse-grained molecular dynamics simulations to delineate the conformational landscape of NLRP3, revealing ligand-dependent allosteric shifts, remodelling of protein–protein interaction surfaces, and determinants of higher-order inflammasome assembly. Supervised ML classifiers trained on features distilled from the simulations robustly discriminated active-like from inactive-like ensembles and predicted the direction and magnitude of inhibitor effects on state populations.

Guided by these computational readouts, we synthesized heterocyclic derivatives that (i) suppress IL-1β release, (ii) reduce pyroptotic cell death, and (iii) attenuate systemic inflammation in cellular and in vivo assays. Selected compounds additionally exhibited blood–brain barrier permeability and neuroprotective activity in mouse models of Parkinson's disease, consistent with on-target modulation of NLRP3-driven neuroinflammation. Collectively, these findings demonstrate that integrating multiscale modelling with machine learning can resolve functionally relevant NLRP3 conformations and accelerate the discovery of allosteric modulators, strengthening the therapeutic rationale for NLRP3 in inflammation-driven pathologies.

INVITED LECTURES

Chemistry area :

X Organic and Bioorganic Chemistry
□ Green Chemistry
□ Material Chemistry
□ Computational Chemistry and AI
□ Medicinal and Food Chemistry

12th French-Italian Chemistry Days
Université Côte d'Azur
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IL-1

Custom-Made Boronium Macrocycles:

An Easy Access to Selective Anion Receptors

Olivier Chuzel

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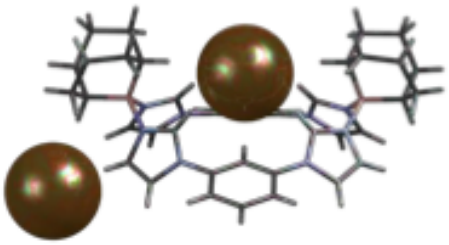
Considering the fundamental role played by anions in biological, environmental and chemical processes, detection, selective recognition and sensing of anions are topics of importance.[1] Consequently, the use of organic ligands with weak non-covalent interactions (e.g., ionic interaction, hydrogen bonds, Van der Waals forces, etc.) is an active field in anion supramolecular chemistry.[2] However, designing highly selective with strong binding affinity receptors for anions is extremely challenging, in part because of large ionic radius, low charge density, and low hydrogen-bonding ability. Thereby, the design of selective anions receptors with high binding associative constant, notably in water, is particularly difficult.[3]
Synthesis and physical properties of an air- and water stable family of bis-cationic macrocyclic imidazolylboronium anion receptors (BIB) will be presented here. By taking advantage of the structure and reactivity of 9-borabicyclo[3.3.1]-nonyl derivatives, boron atom becomes a keystone to offer rigid and highly stable dimeric imidazolylboronium macrocycles.[4] These macrocycles are designed around a functionalized aromatic linker allowing the modulation of physical-chemical properties. Interactions in these anion receptors come in part from several C-H binding sites, including C_{sp^2}-H and C_{sp^3}-H hydrogen-bond donors.



[1] *Anion Coordination Chemistry*, Eds: Bowman-James, K.; Bianchi, A.; García-España, E. Wiley-VCH, Weinheim, **2012**
[2] Zhao, J.; Yang, D.; Yang, X.-J.; Wu, B. *Coord. Chem. Rev.* **2019**, *378*, 415-444
[3] a) Escobar, L.; Ballester, P. *Chem. Rev.*, **2021**, *121*, 2445-2514. b) Dong, J.; Davis, A. P. *Angew. Chem. Int. Ed.*, **2021**, *60*, 8035-8048
[4] a) Toure, M.; Charles, L.; Chendo, C.; Viel, S.; Chuzel, O.; Parrain, J.-L. *Chem. Eur. J.*, **2016**, *22*, 8937-8942. b) Toure, M.; Chuzel, O.; Parrain, J.-L. PCT Int. Appl. (2014), WO 2014206931 A1 20141231

Chemistry area :

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IL-2

How can we shine (sun)light on a more sustainable future?

A physicochemical perspective on the required materials engineering.

B. Bonelli[*]; Nicola Blangetti;[(1)] Najeebullah Channa;[(1)] Michele Bucchieri;[(1,2)] Sara Venturi[(1,2)], Francesca S. Freyria[(1)].

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(1) Department of Applied Science and Technology and INSTM-unit of Torino – Politecnico, Corso Duca degli Abruzzi 24, I-10129 – Torino (Italy).
(2) Department of Chemistry, Biology and Biotechnology, Università degli Studi di Perugia, Via Elce di Sotto 8, Perugia 06123, Italy.

Solar photocatalysis is a sustainable technology that uses sunlight and a semiconductor-based catalytic system to drive chemical reactions, converting solar energy directly into chemical energy. It is primarily used for environmental decontamination, and holds promise for the production of fuels and high-value chemicals [1]. Sunlight is largely unexploited: ca. 95% of photons are in the visible and near-infrared (NIR) regions and cannot be used because most photocatalysts' band gaps require UV light [2]. Doping with heteroatoms is a traditional way to extend the semiconductor bandgap towards the visible range. Still, it introduces undesired defects that, in turn, act as recombination centres, and the Moss-Burstein effect (i.e., an increase in the bandgap energy) at high doping levels. The formation of homo- and heterojunctions helps separate photogenerated electrons and holes. Still, the physicochemical characterization of junction types often requires advanced techniques, which can lead to controversial interpretations. One of the most interesting scientific issues, however, is the exploitation of both the visible and the Near Infrared Range (NIR) in photocatalytic systems capable of upconversion, i.e., a specific physical process by which two low-energy photons are converted into one high-energy photon, which a photocatalyst could in turn exploit. Most upconversion systems currently rely on Lanthanides, but hybrid systems capable of triple-triplet annihilation upconversion could open new possibilities towards solar photocatalysis. Several scientific and technological gaps must be overcome; in this presentation, the issues related to the large bandgap and the rapid recombination of electrons and holes will be addressed from a physicochemical perspective, with an eye toward the use of sustainable materials and green synthesis methods for TiO_2-based photocatalytic systems.

[1] Lei, D.; Wang, L.; Lv, Y.; Luo, N.; Wang, Z. *Chem. Eur. J.* **2024**, *30*, e202401486.
[2] M. Bucchieri, F.S. Freyria. B. Bonelli, *J. Mater. Chem. A* **2025**,*13*, 18115-18145.

Chemistry area :

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IL-3

The Hunt for Impurities

Gregoire Mouis, Mathilde Schembri, Marina Ayubova, Tony Cachot, Thomas Texier,

Kevin Reverse, Thibaud Gerfaud, Arnaud Mathieu, ***Guillaume Tintori,*** ***Jean-Guy Boiteau****

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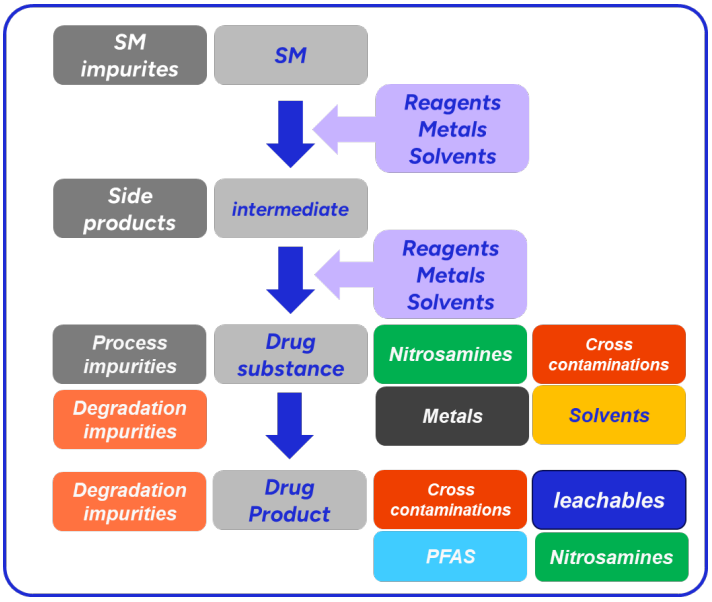
The detection of impurities in active ingredients (API) is essential to ensure patient safety, as certain impurities can be toxic, genotoxic, or cause adverse effects even at very low levels. Furthermore, this approach meets international regulatory guidelines that mandate the identification, quantification, and control of organic, inorganic, and volatile impurities throughout the product life cycle.
Impurities can come from raw materials, be generated by side reactions or degradation reactions, or result from cross-contaminations. Identification by HRMS, isolation by preparative HPLC, and characterization by NMR enable us to identify their structure and understand their formation mechanism. Through several examples encountered, we will explore this surprising chemistry.



[1] **Identification of specified and unknown impurities J, K, L and RRT 2.6 and 3.4 in Tetralysal® capsules** Billié, S.; Reversé, K.; Cachot, T.; Mouis, G.; Pierre, R.; Chambon, S.; Gerfaud, T.; Longoni, D.; Raynard, H.; Charras, K.; Bertin, D.; Boulier, A.; Trognon, C. ; Zanelli, U.; Furnes, B.; Boiteau, J-G. ;* Harris, S. C.* *Eur. J. Pharm. Sci.* **2023**, *188*, 106519
[2] **Completion of the Impurity Profile of Lymecycline : Formal Identification of Impurities E and F** Billié, S.; Reversé, K.; Chambon, S.; Cachot, T.; Pierre, R.; Gerfaud, T.; Longoni, D.; Gennari, M.; Raynard, H.; Talbot, E.; Charras, K.; Bertin, D.; Joly-Battaglini, Pedrassi, G.; Boiteau, J-G.; M.; Cren, C.; Harris C. S. *J Pharm Biomed Anal*, **2022**, *220*, 114993-11505.

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IL-4

Capturing DNA lesions (photo)chemistry in silico

Dumont, E.*

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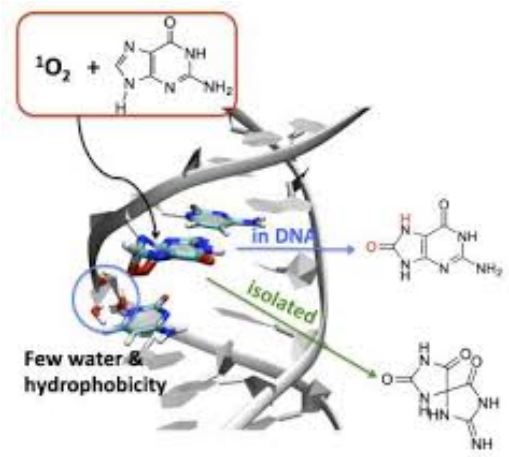
DNA is a well-celebrated double-stranded helix ensuring genomic integrity yet constantly exposed to light and reactive oxidatively-generated species. The latter can give rise to either simple or so-called complex DNA lesions, detected by HPLC/MS-MS(-MS), with an underlying combinatorial chemistry.

Reyling on classical molecular dynamics with tailored force field parameters, eventually coupled to quantum chemistry, it is possible to generate plausible structures of damaged oligonucleotides up to the nucleosomal scale and corroborate these findings against experimental evidences.

DNA-photosensitizers interactions can also be probed computationally which consolidates over the years a predictive, Alphafold-like dynamical computation protocol. I will exemplify the role of molecular modeling to guide the design of enantio-selective photoDNAzymes [1].



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IL-5

Exploring the pharmaceutical potential of highly substituted pyrazoles: from chemical design to antitumor activity

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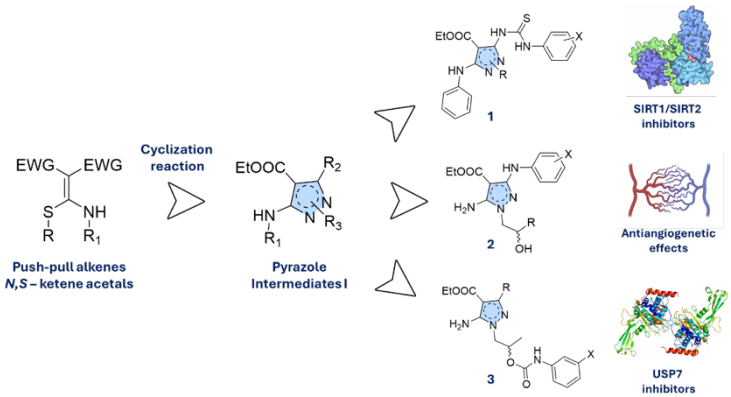
The pyrazole nucleus represents a privileged scaffold in medicinal chemistry being shared by several pharmaceutically relevant compounds with a broad range of activities [1]. In the last years, we developed novel synthetic procedures for the synthesis of highly functionalized amino-pyrazole derivatives starting from the versatile *N,S*-ketene acetal frameworks [2,3]. The cyclization reaction of these push-pull alkenes with the proper substituted hydrazine allowed us to isolate pyrazole intermediates **I**, differently functionalized on the heterocyclic core. Based on the structure-activity relationships (SARs) of the previous reported molecules, intermediates **I** were suitably converted into pyrazoles **1-3** through different stepwise procedures. The obtained derivatives were fully characterized and tested for their antitumor activities. More specifically, pyrazolyl thioureas **1** showed micromolar IC_{50} against Sirtuin 1 and Sirtuin 2, phenylamino pyrazoles **2** displayed antiangiogenetic activities by stabilizing IGFBP-4, while pyrazole carbamates **3** proved to inhibit USP7 deubiquitinating enzyme. The synthetic procedures, the characterization of the compounds as well as the biological results will be discussed during the presentation.



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ORAL COMMUNICATIONS

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COM-1

A new catalytic methodology to access oxepane derivatives, from 1,5-diepoxides, for therapeutic applications

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Cancer remains one of the leading causes of death worldwide and continues to represent a major challenge for medicinal chemistry.[1] In particular, hypoxic tumors are associated with poor prognosis due to their strong resistance.[2] The discovery of new bioactive scaffolds able to overcome this therapeutic resistance is therefore a key issue of the research in therapeutic chemistry.

Marine natural products represent an untapped reservoir biologically active compounds, highlighting highly complex scaffolds. Among them, sodwanone A, a triterpenoid isolated from the marine sponge *Axinella weltneri*, has attracted attention due to its ability to inhibit the activation of the hypoxia-inducible factor HIF-1.[3] Structure of sodwanones includes an oxepane ring, a seven-membered cyclic ether mostly found in marine natural products.

Cyclic ethers containing five to seven-membered rings are widely represented in marine natural products with significant biological activities. Their formation remains an important challenge in organic synthesis, particularly due to the unfavorable entropic factors associated with medium-sized ring formation. Among the different strategies developed to access such structures, epoxide-opening reactions have proven to be a potential approach for the construction of cyclic ethers.

Such transformations are usually performed under stoichiometric conditions. Lewis superacids provide an efficient catalytic alternative to activate oxiranes and promote biomimetic intramolecular cyclization cascades. In this context, we investigated the reactivity of terpenoid polyepoxide substrates, with a focus on the catalytic cyclization of 1,5-diepoxides. Activation of these substrates by metallic triflates, especially $Bi(OTf)_3$, triggers epoxide-opening cascades that selectively generate oxepane derivatives, with diastereoselectivity influenced by the substrate stereochemistry.

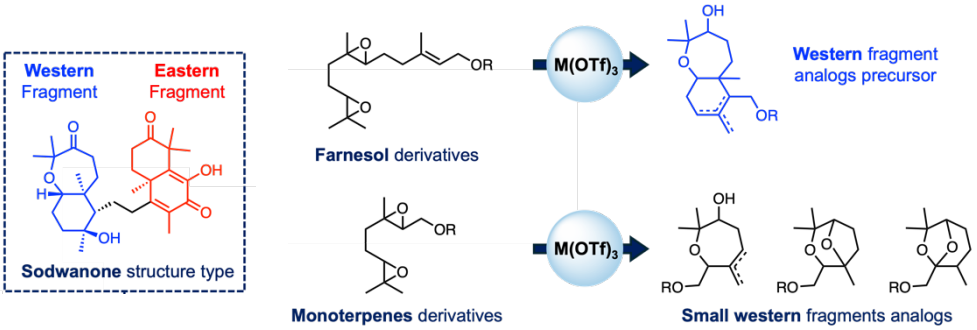

Figure 1 : Overview of the project

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COM-2

Aqueous Binary Deep Eutectic Solvents (aquoDESs) as effective and Environmentally Friendly Reaction Media for the Wittig Olefination

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The Wittig reaction[1] is a reliable method for alkene synthesis, enabling the chemo-, regio- and stereoselective olefination of carbonyl compounds through phosphorus ylides.[2] Owing to its versatility and broad substrate scope, this transformation is widely used in academia and industry.[3] Wittig olefinations are usually carried out in dry, aprotic solvents, under homogeneous conditions, and often require strong bases for ylide generation. In search of more sustainable alternatives, several modified Wittig protocols have been developed in recent years.[4] In our previous work, we showed that Deep Eutectic Solvents (DESs) are suitable media for greener Wittig olefination, although solvent recovery and reuse remained challenging.[5]

Building on these results, we extended this strategy to water-based eutectic systems (aquoDESs) because of their low toxicity, reduced viscosity and potentially improved recyclability.[6] Different aquoDESs were investigated as media for the Wittig reaction by screening bases with different basicity at room temperature and in air. These systems proved effective for the transformation, affording the desired olefination products in good yields, with weak bases emerging as the most efficient promoters. Notably, the solvent could be recovered and reused over several cycles without loss of reaction efficiency, further enhancing the sustainability of the protocol.

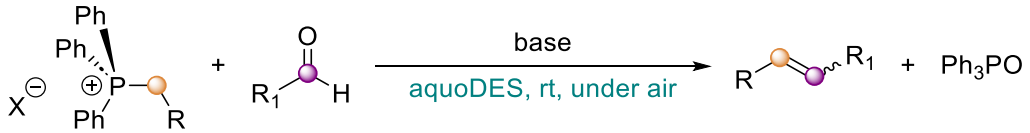

Figure 1: Wittig olefination in aquo-DES.

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COM-3

Development of new triazoles triggering apoptosis and ferroptosis for leukemia treatment

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Acute leukemias represent one of the most common malignant disorders. Recently, targeted therapies made real breakthroughs in Chronic Myeloid Leukemia (CML) and Acute Myeloid Leukemia (AML) treatments, drastically improving survival rates.[1,2] Most of the drugs used in these targeted therapies are tyrosine kinases inhibitors (TKIs) targeting BCR-ABL or FLT3) and IDH or BCL-2 inhibitors. These drugs mainly induce cell death through apoptosis and are subject to resistance, thus limiting their efficacy.[1,3] Recent studies highlighted ferroptosis as a promising strategy to cause cell death. Our work focuses on the development of new inhibitors that trigger AML cell death through both apoptosis and ferroptosis, aiming to overcome therapeutic resistance.[4] Two compounds, a nucleoside (231) and a non-nucleoside analogue (HA344), have shown strong activity against CML K562-S cells (Figure 1). We recently identified GPX4 and TXNRD1 as targets through a click chemistry approach coupled to mass spectrometry.[4] Despite strong *in vitro* activity, these compounds suffer from short half-life *in vivo* due to fast ester hydrolysis. Consequently, our recent work focuses on replacing these ester moieties to improve *in vivo* stability. Additionally, we are pursuing a Structure-Activity Relationship (SAR) study, designing new analogues, to improve GPX4 and TXNRD1 inhibition.

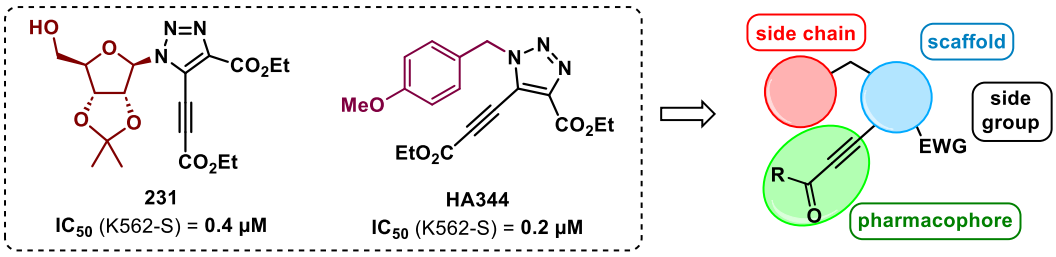

Figure 1. Structure, activity and SAR map of triazole analogues 231 and HA344

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COM-4

Stereoselective addition of aromatic dithiols to Levoglucosenone and their application in polymerization

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Levoglucosenone (LGO; 1,6-anhydro-3,4-dideoxy-β-D-glycero-hex-3-enopyranos-2-ulose) is a valuable biobased platform molecule derived from cellulose waste materials such as sawdust via a simple acidification and pyrolysis process[1]. Its synthetic utility derives primarily from the presence of an enone functional group and a cyclic acetal bridge, both of which readily participate in addition, substitution, and ring-opening reactions[2]. Because many of these transformations proceed with high stereoselectivity to afford single diastereomers, LGO has been widely utilized as an important chiral building block in various research fields, including pharmaceutical science and the total synthesis of natural products. Although reports on stereoselective polymerization using LGO remain limited, the formation of tricomponent polymers composed of LGO, 1,4-benzenedithiol, and dicarboxylic dihydrazides was recently described[3]. In these systems, complete stereochemical control was achieved, yielding exclusively the exo configuration for the C–S bond and the E configuration for the C=N bond. Here, we report the novel synthesis of LGO-based monomers linked with 1,3- and 1,2-benzenedithiols as alternatives to 1,4-benzenedithiol and their subsequent polycondensation (*Fig.1)*. The resulting polymer properties were investigated and compared, focusing on thermal and optical features of the obtained materials. The degradability of the final products was also evaluated. Furthermore, when possible, harmful solvents and procedures were replaced by safer alternatives.

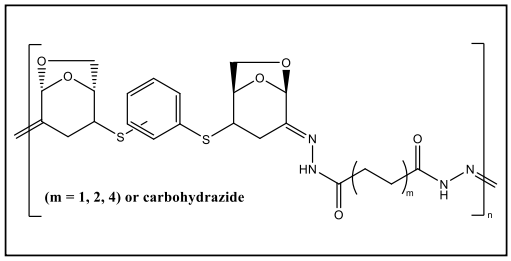

Figure 1: Generic structure of the obtained polymers

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COM-5

Accessing 2,3-Fluoroalkynylated *N*-heterocycles *via* Gold Catalysis

Baubiat, E.(1); Lubrano Di Scampamorte, L.(1); Olivero, S.(1); Melot, R.(1)*; Michelet, V.(1)*

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Among natural products and active compounds, nitrogen-containing heterocycles - pyrrolidines, piperidines, and azepanes - play a crucial role as core motifs.[1] To access novel candidates with improved therapeutic profiles, modifying existing structures is particularly valuable. Fluorine introduction can improve metabolic stability, lipophilicity, and bioavailability,[2] while alkynylation provides a handle for further derivatization.[3] Although these two reactions have been well-described independently, a one-step fluoroalkynylation remains under-explored and limited to aryl-alkenes substrates.[4]

In this context and following our endeavor towards gold-catalyzed access to *N*-heterocycles,[5] we embarked on the development of a gold-catalyzed fluoroalkynylation reaction applied to 2,3-unsaturated *N*-heterocycles. This transformation was optimized and was made possible by the use of Selectfluor as electrophilic fluorinated agent combined with the nucleophilic addition of a terminal alkyne activated by a gold complex.[6] This approach gave rise to the diastereoselective preparation of unprecedented 2-alkynyl-3-fluoro-*N*-heterocycles. This presentation will show the latest results on sustainable access to functionalized heterocycles.

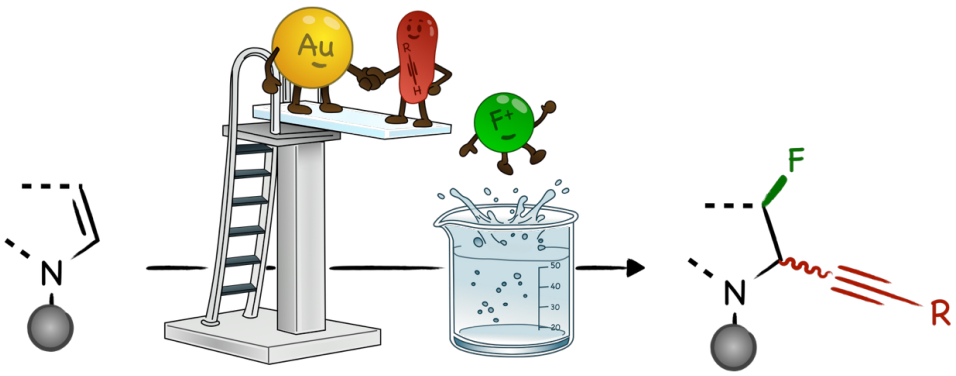

Figure 1 : Gold-catalyzed fluoroalkynylation reaction

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COM-6

Use of *ortho*-quinones in the synthesis of highly functionalized photocycloaddition products

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In this communication, we report a study on the reactivity of *o*-quinones in visible light-driven direct Paternò-Büchi photocycloadditions[1], involving captodative olefines *Z*. These specific olefines are efficiently synthetized via photochemical multicomponent processes, namely the Passerini-like K-3CR and its sylilated version, SK-3CR (***Figure 1(A)***)[2],[3]. The cycloaddition affords highly functionalized compounds with polycyclic aromatic patterns in the structure (***Figure 1(B)***).

Experimental results highlight a significant divergence in the reactivity between quinone **1** and quinone **2**. The structures of the resulting adducts were unambiguously confirmed by X-ray diffraction (XRD) analysis. Furthermore, mechanistic hypotheses for the observed pathways are proposed, drawing on established literature and the unique electronic nature of the substrates.

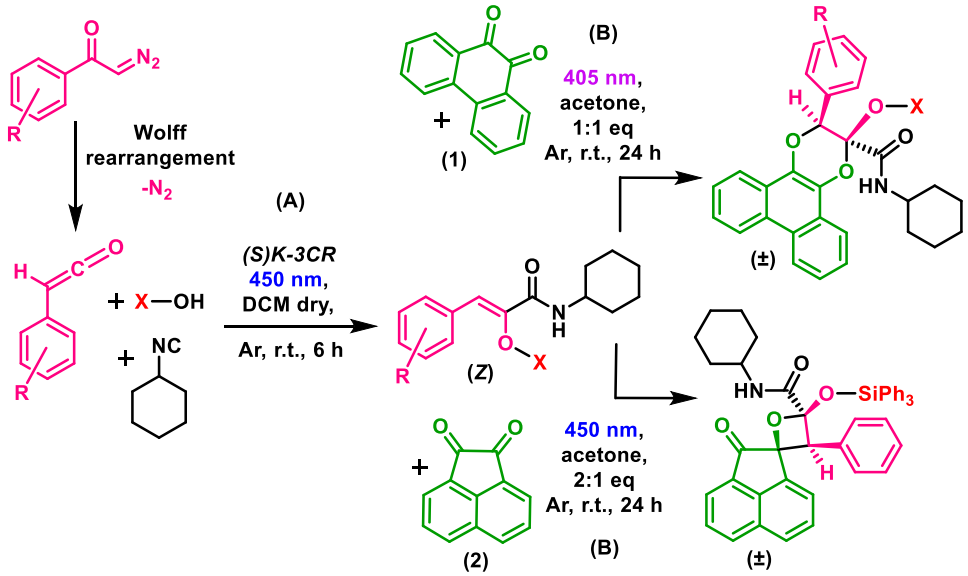

Figure 1. Synthesis of the captodative olefine through a "K-3CR" Passerini-like reaction (A) and photocycloaddition (B) with o-quinones (phenantro-9,10-quinone (1) and acenaphto-1,2-quinone (2)).

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COM-7

Experimental and theoretical investigation of Li_2Se, Na_2Se and K_2Se

Guerrucci, S. (1); Delsante, S. (1,2); Freccero, R. (1); Spaggiari, G. (3,4); Piccinni, M. (1,4); Lodola, F. (5); Mas Garcia, J. (6); Colombara, D. (1)

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(3) Institute of Materials for Electronics and Magnetism, CNR-IMEM, Parma, Italy

(4) Istituto Italiano di Tecnologia, (IIT) Genoa, Italy.

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Alkali elements are known to play a crucial role in improving the performance of CIGS ($Cu(In,Ga)Se_2$) solar cells,[1] although the mechanisms behind their effects are not yet fully understood. This has motivated interest in the study of alternative alkali-containing compounds, such as alkali selenides, which could be used as precursors or doping agents in future device applications. This study focuses on the synthesis and characterization of Ak_2Se, to gain a deeper understanding of their structural, optical, and thermodynamic properties. These compounds were synthesized using reactive flux synthesis[2], which unexpectedly yielded shiny, colorful crystals. This unusual appearance led to further investigation through Raman spectroscopy, photoluminescence (PL), and UV-Vis spectroscopy, supported by *ab initio* calculations and simulated Raman spectra. Complementary characterizations were performed using powder X-ray diffraction (XRPD) and scanning electron microscopy with energy-dispersive X-ray spectroscopy (SEM-EDS), confirming the expected phases and allowing us to monitor their degradation upon exposure to air.

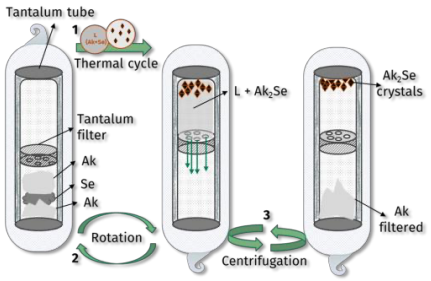

Figure 1 : Experimental setup designed for reactive flux synthesis.

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COM-8

Synthesis, Characterization and Photocatalytic Activity of Bismuth Vanadium Oxides with Various Morphologies

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Bismuth vanadate ($BiVO_4$) is a promising material for photocatalysis and photoelectrochemical (PEC) water splitting due to its excellent visible-light absorption (E_g = 2.4 eV), favorable band edge positions, chemical stability and non-toxicity. However, $BiVO_4$ activity suffers from high rate of charge recombination with small diffusion length (L_h ≈ 70 nm) and slow surface kinetics[1], highlighting the importance for a better control over the size and exposed crystallinity. We demonstrate a facile microwave-assisted solvothermal synthesis, using sodium oleate as shaping agent, yielding various morphologies (micro- and nanorods and nanoparticles). Prior to testing these candidates for PEC water splitting, we evaluated their activity through the photodegradation of methylene blue (MB). In Figure 1, morphology can be assessed in (a), (b) and (c). An overview of the crystal structure (d) of the materials synthesized is provided, ranging from standard monoclinic $BiVO_4$ to bismuth-rich $Bi_4V_2O_{11}$ structure. Insights on ligand exchange will also be presented (Fig.1 e & f), as a critical step to unlock the full potential of these nano-objects by substituting the native oleate functionality with hydrophilic ligands[2] (e.g., citrate, fumarate or oxalate). The MB photodegradation will act as a screening test to validate the ideal combination of morphology, size, crystal structure and ligand exchange maximizing the photocatalytic efficiency of our materials. We demonstrate successful ligand exchange, evidenced by the improvement in particle dispersion. This work showcases strong insights into the ligand-dependent kinetics after substituting the native oleate passivating agent (Fig.1 g). The impact of this substitution is further observed through enhanced MB adsorption under dark conditions, leading to improved photocatalytic activity.

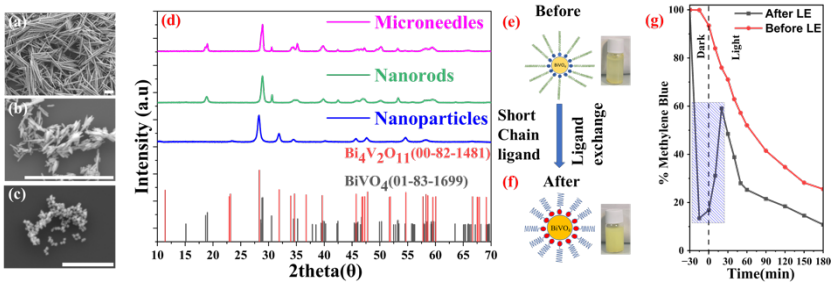

Figure 1: SEM image of (a) microneedles, (b) nanorods and (c) spherical nanoparticles (Scale bar:1µm); (d) XRD of respective particles; (e) and (f) Illustration of ligand exchange (LE) of $BiVO_4$ nanorods particles suspension in water before and after LE. (g) Photodegradation of MB with nanorods before and after ligand exchange (The shaded region highlights the adsorption/desorption kinetics, which is under investigation).

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COM-9

Simultaneous One-Step Formation of Carbon Submicron Fibers and Gold Nanoparticles from Maltodextrin Electrospun Mats

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The polymer industry is still strongly dependent on petrochemical sources and the exploitation of fossil resources. However, since these resources are limited and pose environmental concerns, the development of renewable and sustainable alternatives is increasingly important. Maltodextrins represent a promising option, as they are water-soluble compounds obtained from starch hydrolysis with a dextrose equivalent (DE) lower than 20. Due to their low cost and bio-based origin, they are widely employed, particularly in electrospinning applications.[1] At the same time, metallic nanoparticles have attracted significant interest as catalysts for biomass valorization, contributing to the more sustainable production of chemicals and fuels. Among the different strategies, oxidation processes of biomass, especially those involving polyhydroxylated biomass-derived molecules, are particularly appealing, as they can be converted into high-value products such as aldehydes, ketones, and carboxylic acids.[2] For these reactions, heterogeneous gold-based catalysts are commonly used because of their high catalytic activity and selectivity. These nanoparticles are generally dispersed on porous supports to maintain the active phase well distributed. Among various supports, amorphous carbon is the most widely used due to its large surface area, high porosity, and low cost.[3] In view of the need to replace petroleum-derived precursors in activated carbon production, this work aims to demonstrate the preparation of gold nanoparticle catalysts supported on carbon fibers through a novel one-step method that avoids solvents, external reducing agents, and fossil-based compounds. Solutions containing Glucidex 2®, citric acid, water, and different amounts of tetrachloroauric (III) acid trihydrate were electrospun to produce fibrous mats, which were then subjected to pyrolysis under a nitrogen atmosphere to induce metal reduction and promote the nucleation and growth of gold nanoparticles. The materials were characterized by XRD, SEM, FESEM, and TEM to study the morphology and size distribution of the nanoparticles. The catalytic activity was evaluated by investigating the glycerol oxidation reaction, and conversion was measured by HPLC/UV-vis analysis. The catalyst with the lowest gold loading, exhibiting the smallest average nanoparticle size, showed the highest activity, reaching a glycerol conversion of 45%.

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COM-10

Crosslinkable chromophores for non-linear optic (NLO) applications: design, synthesis and evaluation of NLO properties

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Electro-optical (EO) modulators based on the Pockels effect are widely used in modern telecommunications, AI, quantum computing, etc due to their fast light modulation capability. While commercial electro-optics are mostly based on inorganic materials, organic materials offer several advantages, including broader bandwidth, lower power consumption, smaller device footprint, and potentially less cost. [1]

The bottleneck hampering a wide application of organic NLO materials are relatively high optical losses and insufficient stability at elevated temperatures and optical powers. Thus, the design, synthesis and studying of new materials along with the development of advanced processing protocols for integrating organic electro-optic (OEO) materials into various device architectures, remains of a hot topic. [2]

We propose 2-styryl-chromones (***Chyba! Nenašiel sa žiaden zdroj odkazov.****a*) embedded in epoxy-type polymers as a basic motif for improved organic NLO materials. Monomeric chromophores with similar core have been reported to exhibit high enough hyperpolarizability [3]. The chromophores incorporation into epoxy polymer network via -OH and -NH_2 cross-linking groups we are expecting to further enhance the thermal stability of their NLO properties (***Chyba! Nenašiel sa žiaden zdroj odkazov.****b*).

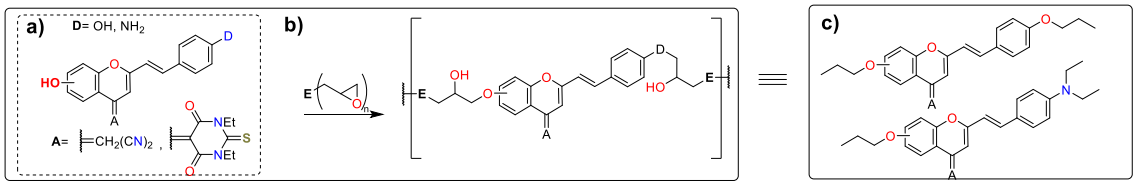

Figure 1 a) General design of 2-styrylchromon chromophores b) Scheme of crosslinking of the chromophores into epoxy polymer c) Alkylated chromophore, serving as a relevant model chromophore

The positions of the cross-linking groups in chromophores were optimized based on DFT calculations of the 1st hyperpolarizability. It's experimental values was obtained by 2nd harmonic generation technique. Satisfactory high experimental values and good accordance with the theoretical ones make promising our approach to the design of NLO chromophores.

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COM-11

Electrochemical behaviour of Cu-, In-, and Ga-based liquid metal salts

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Ionic liquids (ILs) are salts that melt at room temperature or below 100°C. The integration of metal ions into ionic liquids (ILs)—either through solvation or as structural elements—yields a sub-class of ILs known as liquid metal salts (LMSs). Both ILs and LMSs have recently gained rising interest due to their unique physico-chemical properties, such as low vapor pressure, high thermal stability, and nonflammability, electrical conductivity and large electrochemical window [1] [1,2]. These features make them appealing in many applications. LMSs are particularly interesting as electrolytes for batteries, and they have been investigated as new materials for memristors [1,3]. Besides these applications, metal electrodeposition from LMSs for photovoltaics and other fields is a sought possibility. In this contribution, we explored the electrochemical behaviour of three 1-buthyl-3-methyl imidazolium (BMIm)-based LMSs containing Cu, Ga, and In complexes as anions: $[BMIm]_2[CuCl_4]$, $[BMIm][GaCl_4]$, and $[BMIm][InCl_4]$ (Figure 1). Their electrochemical activity was compared with the BMImCl, to isolate the electrochemical processes involving the MCl_4^{n-} anion.

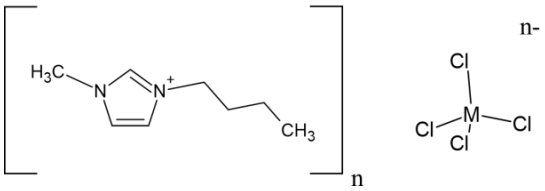

Figure 1 General structure of BMIm-based LMSs.

REMAP has received funding from the European Commission PathFinder Open programme under grant agreement No. 101046909.

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COM-12

Preparation and characterization of Ion-Imprinted Polymer Films for Cadmium(II) Recognition.

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Heavy metal pollution poses serious risks to the environment and human health. Among them, cadmium (Cd^{2+}) is a highly toxic metal ion. Ion-imprinted polymers (IIPs) are selective materials obtained by polymerizing functional monomers around a target ion template. After template removal, specific binding cavities complementary in size and functionality are generated[1]. When fluorescent monomers are used, metal binding can be directly transduced into a measurable fluorescence signal[2].

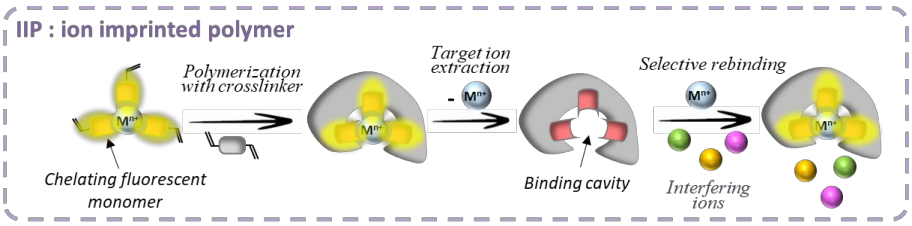

Fig 1: schematic representation of the synthesis of an Ion-Imprinted Polymer IIP based on a fluorescent functional monomer.

In this work, we report the design of a dual-mode chemical sensor for cadmium detection in water, combining fluorescence and electrochemical transduction. A new terpyridine-based fluorescent monomer was synthesized and first evaluated in solution for its Cd^{2+} sensing properties[3].

For electrochemical detection, the monomer was incorporated into surface-grafted IIP films formed directly on pre-functionalized electrodes *via* a "grafting through" polymerization strategy. This approach yields covalently anchored, stable, and reproducible imprinted films.

This strategy opens new perspectives for selective and sensitive dual electrochemical/fluorescent detection of cadmium(II) using innovative functional materials.

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COM-13

A STUDY OF CALCIUM CARBONATE HEMIHYDRATE (CCHH) BY LOW TEMPERATURE SOLID-STATE NMR

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Calcium carbonates ($CaCO_3$) are ubiquitous materials that can be synthesized in the laboratory or found in nature, such as marine sediments, biological organisms, and other systems necessary for various industrial and scientific applications. It has been discovered that $CaCO_3$ exists in three anhydrous crystalline phases ($CaCO_3$) - **Calcite, Aragonite and Vaterite** - as well as two hydrated phases, **Monohydrocalcite** ($CaCO_3.H_2O$) and **Ikaite** ($CaCO_3.6H_2O$). In recent years, another hydrated crystalline form of $CaCO_3$ called **Calcium Carbonate Hemihydrate** ($CaCO_3.\ 1/2H_2O$) has been discovered in nature and under laboratory conditions. [1] [2] Owing to its recent discovery, CCHH has received significant attention from many research groups. Many research questions still remain open, for instance, its crystallographic structure and its formation in biological systems. [3] Understanding the $CaCO_3$ crystallization process allows researchers to move towards a full description of the mechanisms underlying the ACC-to-crystalline phase transition, especially in the context of biomineralization due to its impact on geological environment. In this present research, we focus to investigate the crystallization pathway of this metastable CCHH crystalline phase. Our objective is to shed light on the crystallization pathway of synthetic CCHH at different time points monitored for the first time by using ssNMR spectroscopy in complement with SEM analysis. Our strategy is to employ solid-state Nuclear Magnetic Resonance (ssNMR) to study the sequence of crystallization events at the atomic scale. More specifically, the crystallizing system is rapidly quenched to low temperature at specific time points during crystallization. The crystalline phases present can then be investigated in detail using a range of sophisticated NMR techniques, particularly to quantify the different species present at the different crystallization time points. This work opens up the prospect of studying the early stages of CCHH crystallization, at which traditional characterization techniques may not be efficient.

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COM-14

Mechanical Recycling of Multi Coupled Material Body Seals Based on Thermoplastic Elastomers in the Automotive Industry

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Thermoplastic elastomers (TPEs) are progressively reforming the automotive industry due to their combination of elastomeric behavior, low density, and high recyclability. Unlike conventional vulcanized rubbers, which are permanently crosslinked and difficult to reprocess, TPEs can be remelted and reshaped without significant loss of properties, thus offering a more sustainable and versatile alternative. [1][2] Their use contributes to vehicle lightweighting and, consequently, to reduce CO_2 emissions. [3] A representative example is the substitution of vulcanized EPDM rubber with TPE-based materials in automotive sealing systems.[4] These components are typically multi-material assemblies, combining Thermoplastic Elastomer Vulcanizates (TPV) and Styrenic Thermoplastic Elastomers (TPS) with polypropylene (PP) and flocked polyester. However, their heterogeneous composition hinders conventional recycling due to the complexity of material separation. This study evaluates the mechanical recycling of post-industrial multi-material sealing profiles without prior separation. The recycled material, obtained through granulation and remolding, consisting entirely of 100% recycled material, was characterized chemically and mechanically before and after ageing. Mechanical performance was assessed via hardness, tensile strength, tear resistance, and compression set tests, demonstrating good elastic properties retained also after air ageing. UV ageing tests further indicated satisfactory weather resistance, with no significant color variation. Chemical analyses performed by thermogravimetric analysis (TGA), differential scanning calorimetry (DSC), and ATR-FTIR spectroscopy confirmed the material composition and stability. Overall, the results demonstrate that mechanical recycling of complex, TPE-rich multi-material automotive components is technically feasible and effective. This strategy supports resource efficiency, reduces reliance on virgin polymers, and aligns with circular economy principles for end-of-life vehicle materials.

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COM-15

A novel and versatile therapeutic strategy based on radical chemistry

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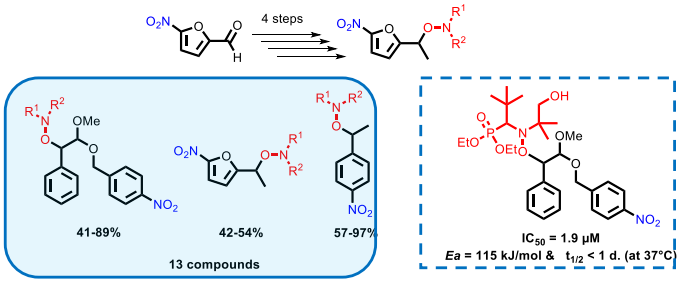
Malaria, leishmaniasis and trypanosomiasis are Neglected Tropical Diseases (NTDs) whose current treatments suffer from drug resistance. In this context, it is necessary to develop new treatments. Unlike the current doxa, *i.e.* inhibition of enzymatic activity, our unconventional approach relies on the normal use of enzymatic activity to release the drug. Our strategy is based on the synthesis of alkoxyamines, which are metastable molecules that homolyze rapidly at 37°C to a stable nitroxide and an alkyl radical. Due to their high reactivity, radicals cannot be administered directly and must be generated *in situ*, close to the site of action. By adding a locker at a key position, alkoxyamines are stable with half-life times reaching weeks or even months under physiological conditions. Lockers are peptide sequences or functions selected to be specifically recognized and activated by parasitic enzymes. Thus, stable locked alkoxyamines are specifically hydrolyzed by parasitic enzymes into highly labile alkoxyamines. An overload of released alkyl radicals induces the death of the parasite due to oxidative stress.

In this project, our goal is to target reductases, essential for the efficacy of antiparasitic nitroaromatic compounds.(b) For this purpose, by attaching a nitro group to an alkoxyamine, we prepared stable alkoxyamines that are activated by selective reduction to produce labile aminoalkoxyamines that spontaneously homolyze.(c),(d) To date, we have synthesized 13 nitro compounds belonging to the family of acetals, styrenes, and furans, using 4-step syntheses, for the treatment of NTDs.(a) Our molecules have been investigated for malaria and trypanosomiasis bioassays, as well as their stability using EPR (electron paramagnetic resonance) analysis to determine their activation energy under biological conditions and their half-life at 37°C. Very encouraging IC_{50} (1.9 µM) values were determined for acetal and styrene structures. With these results already in hand, we are continuing the project with the synthesis of more sophisticated molecular structures, which will then be tested biologically.(e)



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COM-16

From Local Structure to Persistent Luminescence: A PDF and XANES Study of Mn-Doped Halide Double Perovskites

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Persistent luminescence materials (PeLMs) can emit for long periods, ranging from minutes to several weeks, after the excitation source has been removed. This characteristic makes them promising for a wide range of applications such as emergency signage, road safety indicators, bioimaging, photocatalysis, optical data storage, and anti-counterfeiting technologies. In many of these contexts, the use of nanocrystalline PeLMs is necessary; however, reducing the particle size frequently leads to a significant decrease or complete loss of Persistent Luminescence (PeL) at room temperature.[1]

In this study, Mn-doped halide double perovskites were investigated by synthesizing a series of compositions of $Cs_2(Ag_xNa_{1-x})InCl_6:Mn^{2+}$ in the form of single crystals (SC) as well as nanostructures, specifically nanocubes (NC) and nanoplates (NP). Because PeL is closely related to the presence of trapping centers, often associated with local structural defects, additional structural characterization was carried out at European Synchrotron using X-ray Powder Diffraction, Pair Distribution Function (PDF) analysis, and X-ray Absorption Near Edge Structure (XANES) spectroscopy at the Mn K-edge, corresponding to the emitting center. The experimental results reveal a pronounced dependence of PeL behavior on both particle size and chemical composition. By modifying the Ag/Na ratio and the dimension of the samples, local structural variations were detected through PDF analysis – Fig. 1a. Furthermore, XANES measurements show that the pre-edge feature is significantly broader in PeL bulk samples (such as SC x=0.8), suggesting the coexistence of Mn^{2+} and Mn^{3+} oxidation states – Fig. 1b. These results contribute to a deeper understanding of how both composition and particle size affect PeL, improving the performance of perovskite-based PeLMs.

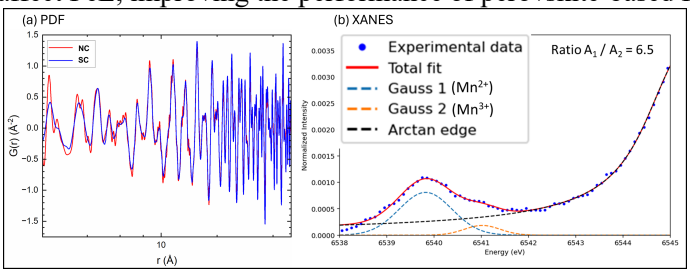

Figure 1 : (a) PDF analysis for NC and SC with x=0.8; (b) XANES spectroscopy at the Mn K-edge for SC x=0.8, detail on the pre-edge, experimental data and fit.

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COM-17

In Situ Radical Formation Induced by Specific Enzymes Triggers Antifungal Activity

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Fungi are eukaryotic micro-organisms widely distributed on Earth, mostly free-living in soil or water, and are of great environmental and medical importance. [a] Some fungi can form parasitic or symbiotic relationships with plants or animals and some of them cause serious diseases in animals including humans and plants. **The development of new antifungal drugs is becoming a public health priority.** [b] Hence, our goal is to design carbohydrate prodrugs that can be activated into highly labile alkoxyamines by secreted enzymes. These highly labile alkoxyamines instantaneously decompose in highly reactive radicals exhibiting random reactivity, inducing the death of fungi as reported with peptide linked to an alkoxyamine. [c]

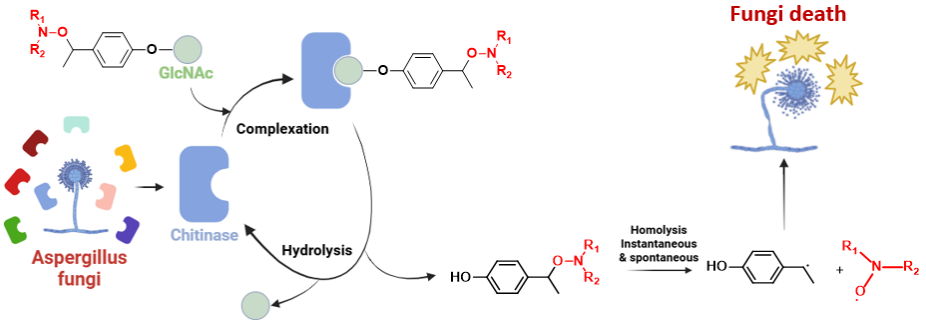

Figure 1: *Enzymatic activation of alkoxyamine vectorized prodrug.*

Our pioneering approach is the synthesis of versatile drugs that can selectively kill fungi in seeds, plants, animals and human beings by using sugar chemistry. Biological investigations of 15 alkoxyamines are ongoing by Pr. David Turra at the University of Naples. [d]

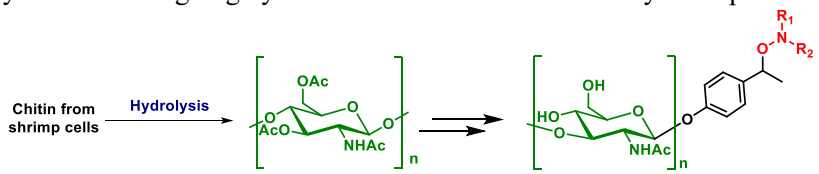

Figure 2: *Targeted vectorized alkoxyamines derived from chitin.*

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[b] Mol. Pharmaceutics. **2014**, 11, 2412.
[c] Journal of Fungi. **2025**, 11, 503.
[d] Publication in progress, redaction.

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COM-18

Mixed-Phase TiO_2 coupled with $CuInS_2$ Quantum Dots for photocatalytic CO_2 reduction

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One of the major environmental challenges in recent years is the reduction of atmospheric CO_2, driving research into artificial photosynthesis to convert CO_2 and water into fuels and value-added chemical under sunlight. Titanium dioxide (TiO_2) is one of the most studied photocatalysts due to its stability, low cost and non-toxicity, however its efficiency is hindered by rapid electron-hole recombination and weak visible-light absorption. Mixed-phase TiO_2 systems have attracted significant interest, as studies on anatase-rutile junction have shown improved band alignment and enhanced charge separation, leading to increased photocatalytic activity [1]. To further enhance light harvesting, TiO_2 can be coupled with $CuInS_2$ (CIS) quantum dots, which feature tuneable band gaps, high absorption, and low toxicity [2]. In this work mixed-phase anatase/rutile TiO_2 was synthesized via a template-free hydrothermal method and compared with commercial benchmark P25. To obtain a sample similar to the P25, the synthesized TiO_2 powder was also calcined at 550 °C. TiO_2 was than coupled with CIS QDs aiming to form a heterojunction capable of extending light absorption into the visible- NIR region and enhances charge separation. XRD analysis confirmed that calcination did not significantly change the phase composition but improved crystallinity, while HRTEM images provided particle size distribution analysis. Coupling TiO_2 with CIS-QDs led to some changes in the textural properties: the specific surface area decreased from ~278 $m^2\ g^{-1}$ (TiO_2) to ~ 145 $m^2\ g^{-1}$ (TiO_2(AR)/CIS), and further to ~ 42 $m^2\ g^{-1}$ for calcined TiO_2(AR)/CIS, while pore volume decreased from ~0.3 $cm^3\ g^{-1}$ to ~ 0.17 $cm^3\ g^{-1}$, and to 0.15 $cm^3\ g^{-1}$.DR UV-Vis analysis revealed an additional absorption band around 600 nm, attributed to CIS QDs which confirm effective coupling and enhanced visible-light harvesting. Preliminary CO_2 photoreduction tests under simulated sunlight showed that the TiO_2(AR)_CALC550/CIS nanocomposite exhibited the highest photocatalytic activity and ethanol selectivity. This fact can be attributed to the synergistic effect of enhanced crystallinity after calcination and efficient interfacial charge transfer within the TiO_2/CIS heterostructure.

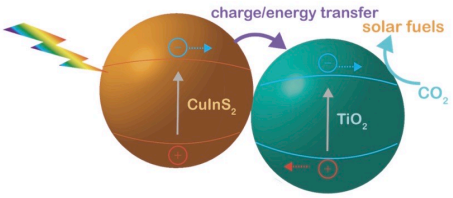

Figure 1: Sketch of the nanocomposite

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Development Of Cu Synzymes Through A Triple Approach: Optimizing The 'Histidine Brace' To Mimic Lpmo Activity

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Biomass represents a sustainable alternative to petroleum-based resources, yet the efficient depolymerization of polysaccharides such as cellulose and chitin remains a major challenge. Lytic Polysaccharide Monooxygenases (LPMOs) address this limitation by catalyzing C–H bond hydroxylation at glycosidic linkages through a mononuclear copper active site coordinated by a histidine brace. However, the precise nature of the copper-oxygen catalytic intermediate is still under debate, and its clarification is crucial to identify the structural and environmental factors that control LPMO reactivity.

The project aims to unravel how the enzyme, the copper ion, and the substrate interact in order to gain deeper insights into the reaction mechanism and further enhance the biopolymer degradation developing smaller catalysts. Thus, we are investigating LPMOs mutants modified in their coordination sphere on the copper center, moving then the attention to smaller compounds aimed to have a mimicking activity, such as short copper-coordinated peptides and small copper complexes made with organic ligands[5]. These two latter kinds of compounds provide access for LPMO mimicking complexes using the so-called “triple-strategy framework”. These studies integrate synthetic chemistry, spectroscopic techniques, X-ray crystallography and spectroscopy (XAS), electrochemical methods, biological tests and DFT computational evaluation. Moreover, a mechanistic investigation carried out by DFT investigation and synthetical intermediate trapping will be fundamental to clarify the cabetalytic pathway and the nature of the actual oxidizing intermediate.

Last but not the least, grafting of active synzymes on molecular supports with cellulose substrate affinity will allow to build up new bionanomaterials coupled with luminescent probes, moving towards a more efficient biomass valorisation throughout a detectable process.

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COM-20

Glass-Ceramic Interactions in Tang Lead-Glazed Ceramics: Insights from Multiscale Synchrotron-based Micro-Imaging Techniques

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Tang lead-glazed ceramics represent a technological achievement of ancient China (618-907 CE), combining complex glaze formulations with controlled low-temperature firing processes. These glassy coatings exhibit strong adhesion to ceramic bodies, acting as protective surface layers, a principle still exploited in modern film technologies [1]. During firing, the molten glaze interacts with the ceramic substrate through cation diffusion and interfacial reactions. Glaze-body interactions and partial melting of ceramic components lead to the formation of newly crystallised interfacial phases, such as Pb-bearing feldspars, $[(K,Ca)PbAl_2Si_2O_8]$. The resulting interfacial microstructures are controlled by ceramic and glaze compositions as well as by firing conditions (time-temperature paths) [2]. Therefore, the glaze-body interface represents a valuable technological archive, preserving physicochemical markers related to raw materials, firing conditions and production practices.

Physico-chemical processes at glass-ceramic interfaces in Tang ceramics remain only partially understood. Spatially resolved, non-destructive micro-imaging techniques are essential to correlate chemical gradients with mineralogical transformations. Here, a multiscale analytical approach integrating laboratory and synchrotron techniques is applied to investigate ceramic-glaze interfaces in both Tang ceramics and modern reproductions. Experiments performed at the European Synchrotron Radiation Facility (ESRF, Grenoble) combined µ-/nano-X-Ray Fluorescence (XRF) and µ-X-Ray Powder Diffraction (XRPD) mapping to characterise interfacial diffusion and stratigraphically resolve phase assemblages, enabling reconstruction of reaction pathways and thermal profiles.

Results reveal complex diffusion patterns and distinct mineralogical reaction layers distinguishing historical from modern samples. SR-µ-/nano-XRF enables quantification of effective diffusion lengths for key cations. The spatial correlation between elemental diffusion and crystalline phases constrains reaction kinetics and firing conditions, providing insights into mechanisms occurring during glaze firing and cooling. The findings highlight the potential of multiscale analytical methodologies for investigating coupled diffusion-reaction processes at glass-ceramic interfaces at the micro- to sub-micrometre scale. This research contributes to a deeper understanding of historical glazed ceramics and provides new physicochemical markers useful for technological interpretation and authentication studies.

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COM-21

Design of bis-electrophilic reagents for the highly chemoselective intramolecular acyl transfer of diamines

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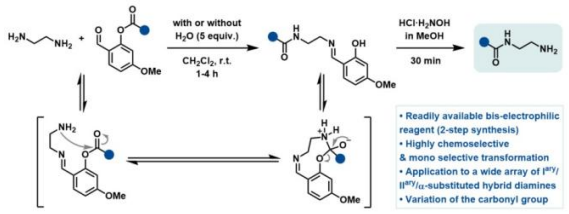
Diamines are widely present in many biologically active pharmaceutical products [1] and natural compounds. [2] They are also a commonly found scaffold in ligands/catalysts for organic synthesis. [3]
The selective mono-functionalization of bifunctional compounds is highly interesting to access such valuable compounds. However, it remains challenging, especially for this type of diamines in which the two amine functions are both highly nucleophilic and difficult to discriminate, thus leading to complex mixtures of mono- and poly-functionalized products. [4] This type of transformation usually requires a passage through protection/deprotection steps, the use of strong acids [5] /bases [6], ie overall drastic conditions. [7]
We propose a new approach for the challenging mono-N-acylation of diamines which takes advantage of an original bifunctional reagent. The latter allows the temporary protection of one amine moiety through the formation of an imine, subsequently leading to the intramolecular transfer of a carbonyl group on the remaining amine moiety. Then, after a simple cleavage of the imine, we can obtain the desired mono-acylated product (Scheme 1). After a thorough optimisation study of the reaction conditions and tuning of the bifunctional reagent, excellent selectivities were obtained between primary, secondary and α-substituted amines, under mild conditions without the observation of any di-acylated product.



Scheme 1. New approach for the selective monofunctionalisation of diamines

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* khadija.ait-moulay@etu-univ-amu.fr; julien.annibaletto@univ-amu.fr

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COM-22

SOLAR ACTIVATED INDIUM-GALLIUM OXIDE PHOTOCATALITYC COATINGS

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Photocatalytic processes aimed at degrading emerging contaminants in water typically rely on powdered wide-bandgap semiconductors such as ZnO and TiO_2. However, these materials often present several limitations, including poor utilization of the solar spectrum, difficulties in catalyst recovery after water treatment, and pronounced light scattering effects that reduce effective photon absorption.
In this study, we report on monolithic photoactive indium-gallium oxide coatings produced through sol-gel route from metal salts. The synthetic procedure is extremely simple and consists of depositing a precursor sol by spin coating or dip coating on a rigid substrate, followed by annealing on a hot plate or by flame treatment. This approach ensures lower energy consumption and better scalability with respect to standard furnace treatments commonly used for similar systems.
We demonstrate that, by tuning the gallium-to-indium ratio, it is possible to control the optical and electrochemical properties of the resulting semiconductor. To assess their catalytic performance, the materials were first tested for the adsorption of different emerging pollutants in aqueous solutions. Subsequently, photocatalytic degradation experiments were conducted under solar simulator irradiation, enabling the investigation of the catalytic processes under realistic operative and illumination conditions.
The monolithic architecture eliminates the need for catalyst recovery and significantly reduces light scattering losses. Gallium oxide provides a wide bandgap and high reduction potential, while the presence of indium enables fine adjustment of the electronic structure, extending the absorbance spectrum over the visible range, and making the system promising for solar-driven excitation.

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COM-23

Molecular approach of uranium and neptunium accumulation in the byssus of *Mytilus galloprovincialis*

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(1) *Institut de chimie de Nice ICN UMR7272 CNRS Université Côte d'Azur, 06108 Nice, France*
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In the event of a nuclear accident or radiological crisis, coastal waters play critical role in the dispersion and trophic transfer of metallic radionuclides, where they are introduced into biogeochemical cycles[1]. Uranium and neptunium (U & Np), central actinides in the nuclear fuel cycle, become bioavailable in seawater and may be transferred to marine organisms[2].
This work aims to first identify the biomacromolecules interacting with actinides in a bioindicator organism[3], *Mytilus galloprovincialis*, and second to elucidate their binding, and possible transfer, mechanisms. After *in vivo* exposure, uranium(VI) speciation with X-ray Absorption Spectroscopies highlighted the mussel foot proteins family (*mfps*) as uranium binding target. *Ex vivo* exposure showed a passive sorption mechanisms, following a linear adsorption behavior at environmentally relevant concentrations. *In vitro* XAS experiments using commercial *mfp-1*, along with a chemical analog (polyethylene glycol functionalized with DOPA residues, PEG-DOPA) evidences the coordination of uranium through oxygen donor ligands, consistent with the catechols in *mfp-1*. After *in vitro* exposure to neptunium(V), UV-Vis-NIR spectrophotometry and XANES both revealed partial reduction to Np(IV) in the presence of *mfp-1*, while PEG-DOPA induces no such reduction, suggesting the presence of redox-active moieties in *mfp-1* (Fig. 1). Overall, this integrative *in vivo - ex vivo - in vitro* approach elucidate two actinide complexation mechanisms, redox behavior, and accumulation pathways in *Mytilus galloprovincialis*. . It provides key bioinorganic insights into the ecotoxicology of uranium and neptunium in marine ecosystems, contributing to improved environmental monitoring and risk assessment following nuclear incidents.

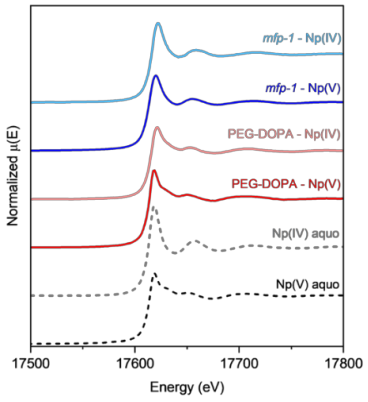

Figure 1. XANES spectra of PEG-DOPA and mfp-1 exposed to Np(V) and to Np(IV), references of aqueous Np(V) and Np(IV).

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Towards Greener Sediment Analysis Using Repurposed Coffee Machines

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The analysis of marine sediments represents a fundamental approach for assessing anthropogenic pressures on aquatic environments, as sediments act as long-term sinks for a wide range of contaminants. These substances can accumulate within sediment matrices and may be released back into the water column under changing environmental conditions, potentially affecting ecosystem health [1]. In recent years, emerging contaminants (ECs) have attracted increasing attention due to their presence, widespread use and limited regulatory control, making their reliable determination in sediments particularly relevant [2].
Traditionally, contaminant extraction relies on techniques such as ultrasonic bath extraction (US), often combined with additional clean-up procedures. While analytically reliable, these methods are generally characterised by high solvent consumption, long extraction times and limited flexibility in the adjustment of key operational parameters [1]. Repurposing devices originally designed for everyday use offers an innovative and cost-effective alternative. Domestic coffee makers, such as the Moka pot, enable solid-liquid-vapor extraction under elevated temperatures and moderately high pressures [3]. However, conventional Moka pots provide limited control over extraction conditions. To overcome this limitation, the present study investigates the application of a Moka-like coffee machine, the Kamira, which allows improved control of solvent volume and extraction parameters while achieving complete extraction in a reduced time (30-40 seconds) [4].
A comparative evaluation of three extraction techniques (US, Moka-pot and Kamira extraction) was conducted using Antarctic marine sediments from Banca Campioni Ambientali Antartici. The Kamira approach showed better performance and was identified as the most suitable method for further optimisation. Extraction parameters were subsequently optimised using a mixture process design, evaluating both process variables (solvent-to-sample ratio and acid concentration) and mixture variables (solvent composition). The results indicated that mixture variables were generally more influential and that the optimal extraction was achieved with an ethanol-water solvent mixture. This method represents an innovative and sustainable alternative for sediment analysis by significantly reducing solvent consumption, extraction time and energy demand. Overall, the approach offers a simple, low-cost and environmentally friendly solution for monitoring ECs in sensitive ecosystems.

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Locking Gd(III) Coiled Coils: Boosting Stability and Relaxivity via Chemical Cross-Linking

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NB: Author who will be present should be written with bold and underlined characters

Coiled coils represent a versatile class of protein-inspired ligands ideal for creating metal binding sites with well-defined sequence-structure relationships.[1-2] However, their practical utility, particularly as Gd(III)-based magnetic resonance imaging (MRI) contrast agents, is often limited by poor stability under physiological conditions. Low kinetic and thermodynamic stability poses a risk of toxic Gd(III) ion release, hindering clinical translation. To address this issue, we employed a strategy based on covalent isopeptide cross-linking, designed to stabilize the hydrophobic core of the protein assembly.[3] The introduction of this cross-link in the Gd(KH2-20X) complex not only improves the chemical stability of the tripeptide, but enhances longitudinal relaxivity (r_1) by approximately 30% at clinical magnetic fields compared to the non-cross-linked analogue, Gd(MB1-2) (from 15.3 to 19.6 mM^{-1} s^{-1}). The mechanism behind this enhancement was investigated through ^1H NMRD studies, which highlighted the predominant role of highly constricted second-sphere water molecules. Furthermore, stability tests conducted in vitro on human serum yielded ^1H NMRD profiles nearly identical to those obtained in aqueous solutions, confirming effective Gd(III) retention and a lack of significant non-specific interactions with serum proteins. Taken together, these results highlight the vast potential of cross-linked coiled coils as a class of MRI contrast agents. The combination of their inherent tunability with the robust stability and optimized hydration dynamics demonstrated here paves the way for the design of a new generation of versatile and effective diagnostic tools.

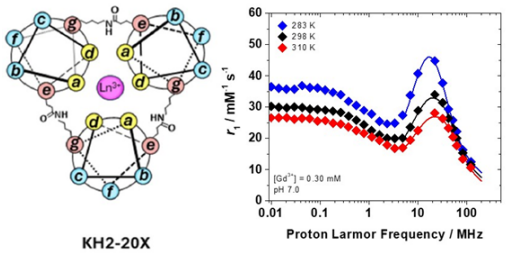

Fig. 1. (Left) Helical wheel diagram of Gd(KH2-20X); (right) ^1H NMRD profiles of Gd(KH2-20X).

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Inhibition of the drug efflux activity of Ptch1 to overcome chemotherapy resistance

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Chemotherapy resistance is responsible for 90% of cancer deaths. Among the various mechanisms involved, the most prominent one is the overexpression of drug efflux pumps that decrease the drug concentration into cancer cells, resulting in the ineffectiveness of treatment. Our team identified the Hedgehog receptor Patched (Ptch1) as an interesting drug efflux pump that participates in the resistance of cancer cells to chemotherapy.[1] Thanks to a screening program, Panicein A hydroquinone (PAH) [2], was identified as an inhibitor of the drug efflux activity of Patched (Figure 1). Indeed, its synthesis allowed us to confirm that PAH increases the cytotoxic effect of several chemotherapeutic agents on melanoma cell lines *in vitro* and *in vivo*.[3]

In this work, we focused on two complementary parts. On one hand, the coupling with a chemical probe, a nitrobenzodiazole(NBD)-PAH analog, to get further comprehension of the mechanism of action via fluorescent labeling. The initial results tend to show that PAH binds to Patched but is not effluxed by it.

On the other hand, the design of a new generation of analogs, derived from our initial hit PAH, has been developed to improve efficacy and physicochemical properties. Therefore, 24 innovative compounds have shown better activity than PAH, in addition to chemotherapy on melanoma cell lines. The most promising one, enabled us to decrease by four the IC_{50} of chemotherapy to reach 12.8µM, and 1.23 of Log D. Moreover, microsomal stability improves the half-time of 1 to 61.5 minutes, which allows us to begin in-vivo assay. Pharmacokinetics study, safety study as well as a mouse in-vivo study have been completed and demonstrate the proof of concept of our lead compound on melanoma cells.

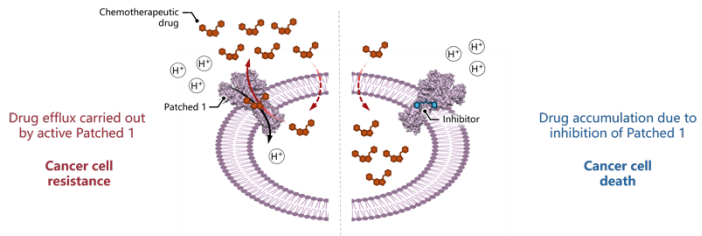

Figure 1 : Representation of the drug efflux activity of Patched and its potential inhibition by small molecules

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COM-27

Engineering Hyaluronic Acid–Lipid Self-Assemblies for Selective Drug Delivery

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Targeting CD44 represents a promising strategy for selective drug delivery in cancer, as this receptor is overexpressed in several tumor types and involved in disease progression [1]. Previous hyaluronic acid (HA) oligosaccharide–PEG–phospholipid conjugates enhanced uptake in CD44-positive lung cancer cells but did not self-assemble, likely due to PEG hydrophilicity [2]. To overcome this limitation, an azido-functionalized HA octasaccharide (DP8) was directly conjugated to dipalmitoylphosphatidylethanolamine (PE) to generate HA-DP8-PE, designed to promote self-assembly while preserving CD44-targeting capability. HA-DP8-PE was synthesized *via* copper-free strain-promoted azide–alkyne cycloaddition under mild conditions, and its self-assembly in aqueous media was evaluated by pyrene fluorescence spectroscopy. The critical micelle concentration (CMC) of 2×10^{-6} M indicated spontaneous nanoassembly formation. The resulting nanoassemblies displayed a mean size below 150 nm and a negative surface charge (−24 mV). Loading with the nitric oxide–donor doxorubicin derivative (DR6) [3] yielded stable nanoassemblies (~110 nm) with high encapsulation efficiency (86%). DR6-loaded nanoassemblies demonstrated enhanced uptake and significantly greater dose- and time-dependent cytotoxicity in CD44-positive lung, pancreatic, and breast cancer cell lines compared to CD44-negative cells. Overall, the HA-phospholipid conjugate forms stable and biocompatible nanoassemblies capable of efficiently encapsulating DR6 and selectively targeting CD44-positive cancer cells, supporting their potential as targeted nanocarriers for cancer therapy.

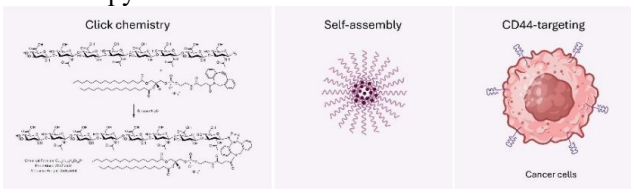

Figure 1: Schematic representation of the formulation strategy

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COM-28

Phytochemical surface corona from Cannabis sativa L. residues modulates the cytotoxicity of green-synthesised silver nanoparticles

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Silver nanoparticles (AgNPs) are extensively investigated for biomedical and environmental applications; however, their cytotoxicity remains a critical limitation. In green synthesis approaches, plant-derived phytochemicals act as reducing and capping agents, strongly influencing nanoparticle surface chemistry and biological behaviour. In this work, we demonstrate that aqueous extracts obtained from *Cannabis sativa* L. processing residues generate AgNPs with unexpectedly low cytotoxicity due to the formation of a protective phytochemical surface corona.

Cannabis inflorescences (WM5, Lavanda CBG, K66/1 varieties) were first subjected to ethanolic maceration for cannabinoid extraction. The residual plant matrix was subsequently extracted with water and used for ultrasound-assisted AgNP synthesis. The tailored synthesis conditions yielded stable, spherical AgNPs with an average hydrodynamic diameter of 43.0 ± 2.6 nm and a ζ-potential of −32.1 ± 0.97 mV. FESEM analysis confirmed monodisperse spherical morphology, while XRPD patterns showed crystalline metallic silver.

Despite physicochemical characteristics comparable to previously reported cytotoxic AgNP systems of similar size, the cannabis-derived AgNPs exhibited remarkably low cytotoxicity in B16-F10, HaCaT, and MCF7 cell lines. Even at concentrations up to 90 µg/mL, no IC_{50} values were observed. This behaviour contrasted sharply with AgNPs synthesised from other plant extracts, including our previous *Ruta graveolens*-derived system.

To elucidate the molecular basis of this reduced cytotoxicity, the cannabis residue extract was characterised by untargeted HPLC–HRMS. The extract displayed a complex composition dominated by polar metabolites and antioxidant phytochemicals, including polyphenols, flavonoids, organic acids, small peptides, and fatty acid derivatives. We hypothesised that this antioxidant-rich phytochemical layer acts as a stabilising and passivating corona, limiting direct metal–cell interactions and modulating silver surface reactivity.

To test this hypothesis, freshly prepared AgNPs were treated with dilute nitric acid to partially or extensively remove surface-bound metabolites. Cytotoxicity increased progressively with increasing acid exposure, and IC_{50} values decreased dramatically across all three cell lines.

FESEM revealed a significant reduction in geometric mean particle diameter after acid treatment (from 49.4 nm to 35.9 nm; $p < 0.001$), while XRPD analysis further demonstrated partial surface oxidation following nitric acid exposure. These findings suggest that the phytochemical coating not only provides steric stabilisation but also protects the silver surface from oxidative transformations that enhance Ag^+ release and cytotoxicity.

Overall, these findings demonstrate that the biological behaviour of green-synthesised AgNPs is strongly governed by the molecular composition of the plant-derived capping layer rather than particle size alone. Cannabis-processing residues, rich in antioxidant metabolites, generate AgNPs bearing a phytochemical corona that attenuates cytotoxicity. This study highlights the importance of controlling extract composition and surface chemistry for the rational design of safer nanomaterials and proposes cannabis industrial residues as a sustainable resource for controlled green nanoparticle synthesis.

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COM-29

Closing the Loop: From Mixed Fish Processing Side Streams to a Pilot-Scale Nutraceutical Formulation

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Global fish production has markedly increased to meet the rising demand for protein- and lipid-rich foods, resulting in greater waste generation and associated environmental impact [1]. Within the Horizon2020 EcoeFISHent project, this study assesses the valorization of unsorted, dehydrated side-streams derived from the filleting of farmed sea bream and sea bass, as well as from canned tuna processing [2].
Several green extraction protocols, including solid/liquid extraction (S/L), microwave-assisted extraction (MAE), supercritical fluid extraction (SFE), and enzyme-assisted extraction (EAE), were investigated at laboratory scale to recover both high-value protein and lipid fractions. Based on Life Cycle Assessment (LCA) and Life Cycle Cost (LCC) studies, EAE was identified as the most scalable methodology. The optimized EAE protocol enabled the simultaneous recovery of protein hydrolysates and fish oils and was subsequently scaled up to a 30 L semi-pilot system, leading to the design and the realization of a 350 L pilot plant to ensure process continuity beyond the project's duration [3].
The resulting protein hydrolysates displayed high purity, a balanced amino acid profile, and a low average molecular weight. The oil extracted from sea bream and sea bass side streams proved to be a valuable source of essential fatty acids and complied with regulatory standards for fish oils, supporting its potential industrial application without requiring further refinement. In collaboration with a nutraceutical-industry partner, a compatibility study was performed to identify suitable formulations for a dietary supplement containing both protein hydrolysates and fish oils (e.g., supplements designed to support sports performance and counteract sarcopenia). Subsequently, several spray-drying microencapsulation trials were conducted, using fish oils (from sea bream/sea bass) in combination with protein fractions extracted from sea bream/sea bass or tuna biomass as wall materials. This integrated approach represents a "closing-the-loop" strategy for a circular economy in the fisheries sector. The aim was to stabilize the bioactive lipid fraction, protect it from oxidation, improve sensory characteristics, and enhance both technological functionality and potential bioavailability, thereby enabling its effective incorporation into nutraceutical formulations.

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Design of New GLS1 Allosteric Inhibitors by the Fragment_Based Strategy

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Glutamine is the second most consumed energy source by cancer cells after glucose, so it has a crucial role in their growth and survival. Glutaminase (GLS1), is associated with cancer cell proliferation in various tumors, particularly with triple-negative breast cancer, being regulated by key oncogenic pathways. Consequently, it has emerged as a high-priority therapeutic target for the development of novel GLS1 inhibitors in oncology. Despite the intense efforts made, to date, only two GLS1 inhibitors (CB-839 and IPN60090) have entered clinical trials. Therefore, in this research, an in silico fragment-based approach is described, aimed at the rational design of new glutaminase allosteric site inhibitors (1).

Forty-seven crystallographic structures of GLS1 are deposited in the PDB. 5HL1 was selected as the most suitable 3D-structure of the target protein. Initial ligand structures for virtual screening were obtained from an in-house dataset of drugs from AIFA and Drug Bank. Docking studies were carried out using Autodock-Vina with the Vinardo scoring function. Then, a fragment-based approach was applied on the best ligands from virtual screening. New molecules were generated through fragments' combination. The process for selecting the top candidates across all three stages (parent drugs, fragments, and newly assembled molecules) was guided by their energy rankings and their ability to conformational match the X-ray binding pose of CB-839, which served as the reference.

Among the known allosteric sites, we focused on the one most widely explored and characterized by structural biology, where CB- 839 and its analogues bind. CB-839 binds within this allosteric region, bridging the two GLS1 monomers. This specific ligand binding mode involves a molecule made up of a "head", a "linker", and a "tail" that can adopt a U-shaped conformation, enabling enzyme inactivation. Considering these factors, a step-by-step docking approach was used to identify initial points to computationally merge the fragments. The top parent drugs were divided into "head", "linker", and "tail" segments, and a fragment library was

implemented. The library was docked into the allosteric binding site to identify the best fragments based on energy ranking and the CB-839 pose overlap. The top solutions from each fragments' group were reassembled to generate new molecules. The final ligands will be docked into the allosteric site. The most promising molecules identified through this approach are undergoing additional validation using molecular dynamics studies, before their synthesis.

Acknowledgments
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Synthesis & Characterization of Novel Gold(III) Complexes via Electrooxidation

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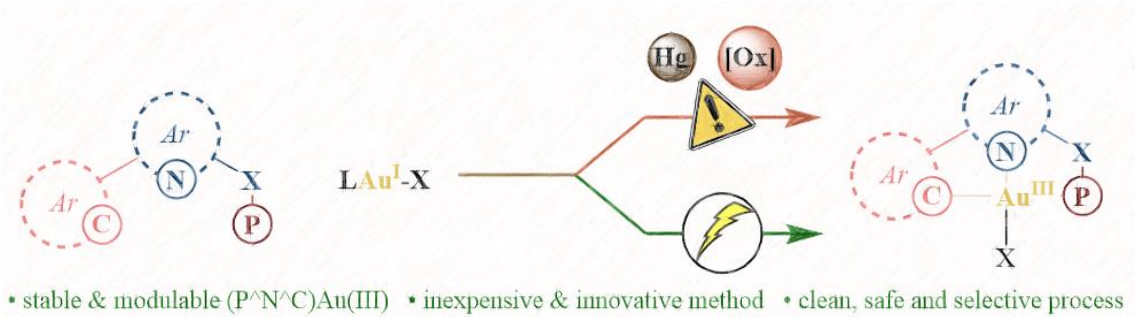
Over the past decades, gold(III) complexes have been shown to be valuable compounds in several research areas such as homogeneous catalysis,[1] medicinal chemistry[2] and optical materials.[3] However, the synthesis of gold(III) species often relies on harsh reaction conditions involving stoichiometric strong oxidants, elevated temperatures or notoriously toxic metals.[4]
In light of the recent reborn of electrosynthesis as a greener and safer alternative to classical oxidants,[5] and inspired by the recent work of C. Nevado's group on *(P^N^C)*gold(III) complexes,[6,7] we developed an efficient access to a new class of *(P^N^C)*gold(III) complexes through the electrochemical oxidation of the easily prepared gold(I) counterparts. This work constitutes an unprecedented, straightforward and original entry to a novel gold(III) platform for the preparation of further valuable gold(III) species.[8]



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Synthesis of Enantioenriched Cyclophanes via Chiral NHC–Palladium-Catalyzed Dynamic Kinetic Resolution

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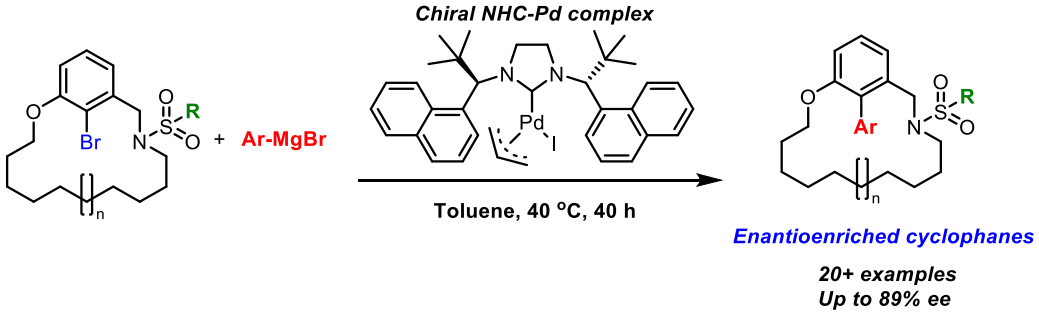
Cyclophanes are intriguing macrocyclic molecules composed of a linker (called *ansa*-chain) connecting two parts of aromatic moiety[1]. Their unique structural characteristics make them valuable in diverse applications, including sensor development, bioimaging, drug delivery, and optoelectronics[2]. Furthermore, suitably substituted cyclophanes can be chiral[3], mostly with planar chirality. In this context, our group synthesized a series of *meta*-cyclophanes and *para*-cyclophanes designed to undergo enantioselective Pd-catalyzed coupling reactions via a dynamic kinetic resolution process. Herein, we will present an enantioselective Kumada-Tamao-Corriu coupling using palladium and chiral N-heterocyclic carbene (NHC) ligands affording *meta*-cyclophanes with up to 89% ee (**Scheme 1**). Our study encompasses the synthesis of cyclophanes, the scope of the reaction, investigation of their configurational stability and applying this strategy to other cross-coupling reactions. This work provides an efficient catalytic asymmetric approach to chiral cyclophanes.



Scheme 1: Pd-catalyzed Kumada coupling affording enantioenriched meta-cyclophanes

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Cryptophane-based Cages Towards Xe/Rn Selective Separation

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Dark matter and neutrinos remain among the most important open questions in modern physics. Their study relies on ultra-sensitive **xenon (Xe)** detectors, a noble gas with excellent detection properties. However, the performance of these detectors is strongly limited by the presence of radioactive **radon (Rn)**, which produces undesirable background signals.[1] Due to their very similar physicochemical properties, separating these two noble gases remains extremely challenging.

To address this challenge, we build on **cryptophane-type molecular cages**, a class of supramolecular containers known for their strong affinity toward Xe and employed in many applications such as ^{129}Xe-MRI sensors.[2] Here, we aim to elegantly tailor new cryptophane derivatives with structural modifications designed to enhance discrimination between Xe and Rn. By tuning the cavity size, shape, and chemical environment of these hosts, we seek to better understand and control noble gas recognition at the molecular level.

The newly developed cryptophanes are then immobilized onto porous solid supports, such as mesoporous silica or MOFs, to generate **hybrid composite materials**. These materials will be characterized and evaluated for their ability to selectively capture radon while maintaining xenon purity at trace concentrations.

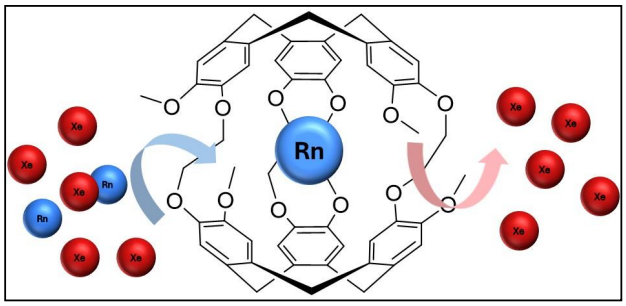

Figure 1: Schematic representation of Xe/Rn separation via cryptophane-based cage.

This work was supported by the National Research Agency (ANR-23-CE31-0022).

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When Snow Reacts: Phase-Controlled Photodegradation of Combustion-Derived Acetophenone

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The widespread presence of organic pollutants in environmental waters also affects cold, rural, and remote regions of the Earth's cryosphere. These areas are not exempt from contamination, as pollutants can undergo long-range atmospheric or oceanic transport and, depending on their volatility, be deposited in snow and ice [1,2]. Beyond acting as cold traps that accumulate contaminants, glaciers and snowpacks are dynamic chemical environments where transformation pathways may differ substantially from those occurring in liquid water [3].

In this work, we investigated the photodegradation of acetophenone (AcPh), a volatile organic compound, emitted to the environment by combustion sources and detected in alpine snow and waters from the Monte Bianco (Italy). Particular attention was given to phase-dependent reactivity by comparing its behavior in artificial snow and in liquid water.

AcPh was identified in alpine snow by UHPLC-HRMS analysis, confirming its occurrence in high-altitude environments influenced by long-range atmospheric transport. Controlled irradiation experiments were then performed on artificial snow at 243 K under UV-A light and compared with parallel experiments performed in liquid water.

Direct photolysis of AcPh was significantly enhanced in snow, whereas it proceeded more slowly in liquid water. The addition of photosensitizers (nitrite, 4-carboxybenzophenone, and anthraquinone-2-sulphonate) to artificial snow did not induce any important indirect photolysis and, in the case of organic photosensitizers, it even inhibited AcPh degradation. In contrast, in liquid water indirect photochemistry prevailed over direct photolysis, particularly in the presence of nitrite and anthraquinone-2-sulfonate.

Experiments conducted with real alpine snow showed lower degradation rates compared to artificial snow, suggesting that natural impurities may inhibit direct photolysis. However, during melting of real snow, indirect pathways became more significant, highlighting the strong influence of phase state and matrix composition on pollutant fate.

Overall, these results shows that snow is not a passive reservoir but an active photochemical medium in which pollutant persistence is strongly controlled by phase-dependent processes. Understanding these differences is crucial for predicting the environmental fate of volatile organic pollutants in cold regions.

Acknowledgements

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Synthesis of materials for Indoor Photovoltaics

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Organic solar cells (OSCs) are light, flexible and inexpensive to produce, with energy conversion efficiencies of up to 19 %[1]. However, they are not widely used for applications with artificial lighting, and their performance is limited, partly due to the use of fullerenes and their derivatives as electron acceptors in the active layer[2]. To overcome these limitations, in this project, we are looking at curcuminoid derivatives to use them as non fullerene acceptors (NFAs). Curcumin is the main molecule of *Curcuma longa* L., also known as turmeric and has been used for centuries as a natural dye[3] and for its medicinal properties[4]. These last decades, curcumin is also studied for its photophysic properties[5] due to its 1.3-diketone core and its π-conjugated skeleton. Curcuminoid derivatives with a difluoron boron difluoride were synthesized to improve the curcumin photophysical properties[6], and are mainly used as fluorescent tags, in optoelectronics[7] like in OLEDs[8], but also in OSCs.
Archet *et al.* [9] synthesized a curcuminoid derivative used as an electron donor in the active layer of OSCs, with power conversion energy up to 4.14 % and a high open-circuit voltage over 1.0 V, when associated with $PC_{61}BM$.
This project focuses on the development of a new family of NFAs: curcuminoid derivatives with a boron difluoride complex, whose structures are inspired by known NFAs. These compounds are synthesized and then characterized (UV-Vis absorbance, cyclic voltammetry, applications in OSCs).

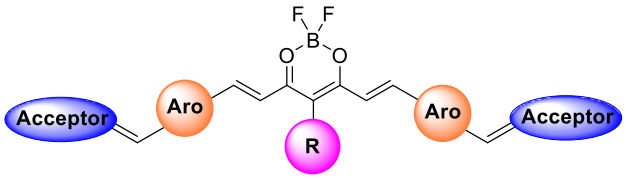

Figure 1 : General structure of curcuminoid derivatives as NFAs

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Activation of small molecules by Frustrated Lewis Pairs

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Catalysis lies at the heart of modern chemical industries, with hydrogenation of unsaturated compounds representing a cornerstone transformation. However, conventional methods rely heavily on transition-metal catalysts, raising issues of sustainability, cost, and environmental impact. As a promising alternative, main-group catalysis based on Frustrated Lewis Pairs (FLPs) has emerged as a powerful concept since 2006[1]. By combining a Lewis acid and a Lewis base that cannot form a stable adduct, FLPs enable the activation of small molecules such as dihydrogen. Despite this remarkable breakthrough, the catalytic efficiency and selectivity of current FLP systems remain far from matching those of established transition-metal catalysts. This limitation underscores the importance of developing new architectures to fully unlock the potential of FLPs in challenging transformation.

This project aims to expand the scope of FLP catalysis by developing ambiphilic architectures 1, in which both Lewis acid and Lewis base sites are integrated into a single molecular framework[2]. Our design relies on an N-heterocyclic carbene (NHC) scaffold bearing a borenium unit as the Lewis acid, complemented by strategically positioned Lewis basic function on the boron atom, the imidazole ring, or near the stereogenic center. This modular design is expected to optimize spatial organization and intramolecular reactivity, providing a versatile platform for enantioselective catalysis.

Ultimately, the objective is to demonstrate that these borenium-based catalysts can split dihydrogen and drive the enantioselective reduction of unsaturated compounds, offering a sustainable, transition-metal-free pathway to asymmetric hydrogenation[3].

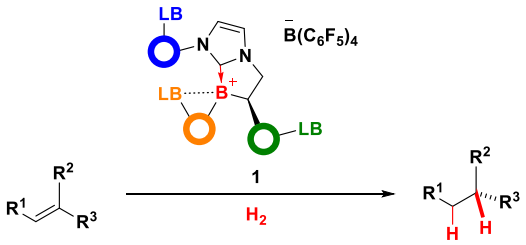

Figure 1: Enantioselective hydrogenation of unsaturated compounds using an FLP catalyst

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P-1

Activation of small molecules thanks to non-metallic radical complexes

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In modern catalysis, the activation of small molecules such as H_2, O_2, and CO_2 is most commonly achieved with transition metals. Although effective, these metals are toxic, scarce, and expensive. In recent years, metal-free strategies based on main-group elements have emerged as powerful tools, with Frustrated Lewis Pairs (FLPs) representing a key breakthrough for small-molecule activation and reduction of unsaturated substrates.[1]

More recently, a radical-based approach has been introduced: Frustrated Radical Pairs (FRPs).[2] Operating through open-shell pathways, FRPs can lower activation barriers and unlock reactivity distinct from classical FLPs.[3]

Our project focuses on developing a novel FRP system combining a Lewis base with a persistent, sterically hindered radical that remains reactive after hydrogen cleavage. In addition, we will investigate how the electronic and steric properties of different Lewis base scaffolds influence the stability and reactivity of these radical pairs under various conditions.

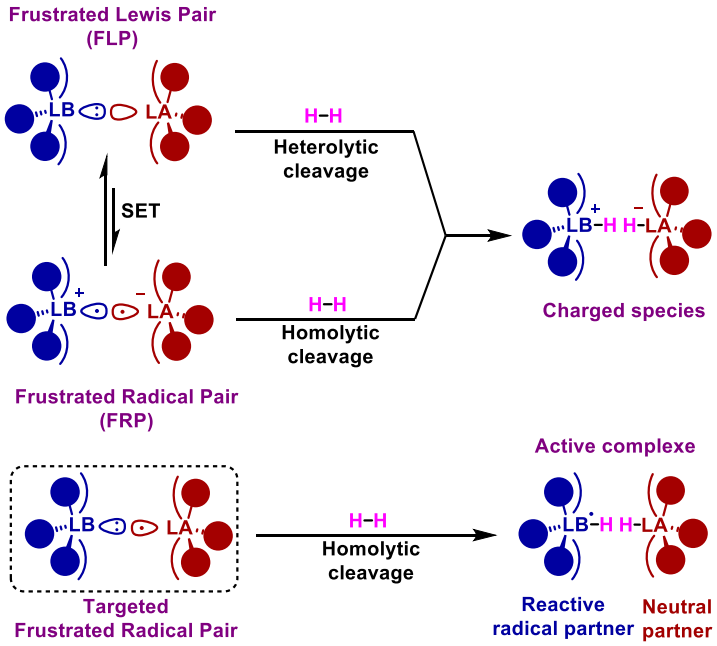

Figure 1: Comparison of classical hydrogen activation by FLPs and the proposed FRP strategy

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P-2

Control of Multiple Stereogenic Elements in Diaryl Ethers

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Axially chiral compounds have received considerable interest from the chemical community due to their great success in the development of chiral ligands or organocatalysts for enantioselective synthesis.[1] Recent advances in atroposelective synthesis have enabled access to diverse atropisomeric diaryl ethers with excellent control of axial chirality. However, the efficient construction of diaryl ethers bearing multiple stereogenic elements axial-central, axial-axial, or axial-planar remains a formidable synthetic challenge.[2] Herein we report a chiral phosphoric acid (CPA)-catalyzed desymmetrizing aminoacetalization strategy of pro-axially chiral dialdehydes that enables the construction of diaryl ethers bearing both central and axial chirality. This organocatalytic atroposelective heteroannulation proceeds under mild conditions, tolerates a broad range of functional groups, and delivers highly enantioenriched products with excellent diastereoselectivity. Kinetic studies revealed a high diastereomerization barrier (141.4 kJ/mol) for representative products, indicating strong configurational stability (Figure 1).[3] This strategy provides a versatile and efficient entry to structurally complex, non-biaryl atropisomers featuring multiple stereogenic elements, thereby expanding the accessible chemical space of axially chiral scaffolds for applications in catalysis, materials science, and medicinal chemistry.

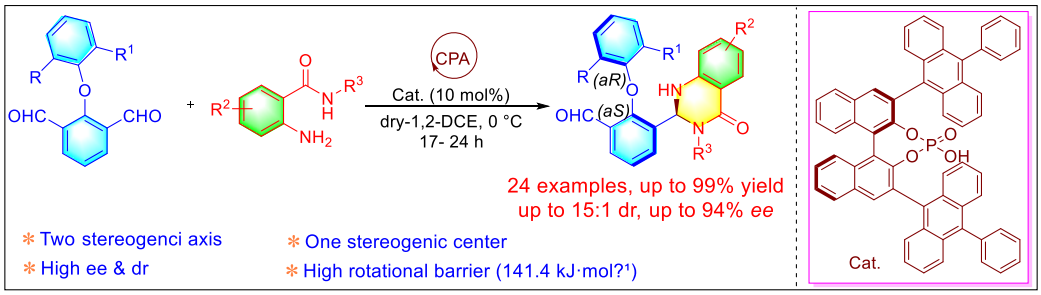

Figure 1: Enantio- and diastereoselective synthesis of multiple stereogenic elements in diaryl ethers.

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P-3

Multicomponent reactions on levoglucosenone

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This study describes the use of levoglucosenone, a bio-based molecule obtained from the selective acid pyrolysis of cellulose-derived materials, as a versatile platform for the synthesis of chiral scaffolds. Levoglucosenone was functionalized via an highly diastereoselective aza-Michael addition with different aliphatic primary amines, affording a series of aminated ketone derivatives. These intermediates (**2**) were stabilized either by amidation[1] of the nitrogen atom (**3**) or by reduction of the unconjugated ketone[2] functionality (**4**) due to their instability[1, 2]. The resulting ketones **2** were then employed in diversity-oriented stereoselective methodologies, such as multicomponent Passerini reactions **5**.[3] The experimental results show high stereoselectivity throughout the synthetic sequence, from the initial Michael addition to the multicomponent reactions. This strategy enables the formation of rigid and complex molecular structures containing up to four stereogenic centers. Overall, this strategy provides access to small libraries of novel enantiopure, three-dimensional sugar-like scaffolds, including structures incorporating peptidomimetic motifs.

We acknowledge financial support under the National Recovery and Resilience Plan (NRRP), Mission 4, Component 2, Investment 1.1, Call for tender No. 104 published on 2.2.2022 by MUR, funded by the European Union – NextGenerationEU– Project Title SUSTCARB – CUP D53D23010360006, - Grant Assignment Decree No. 1064 adopted on july 18, 2023

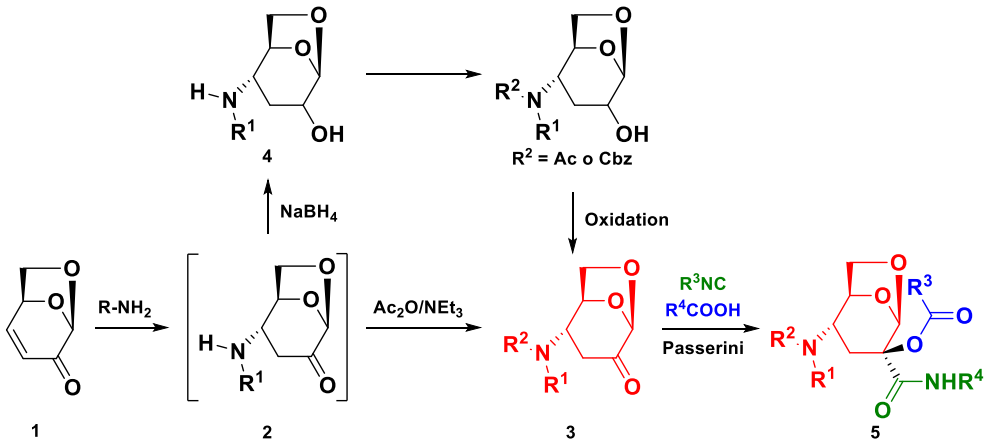

*Figure 1 : Synthetic pathway for the formation of the ketones **3** to use in multicomponent reactions through the aza-Michael addition and the stabilization of the intermediate **2**.*

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P-4

Synthesis of molecular cages based on porphyrin and cycloveratrylene derivatives for enantioselective photocatalysis

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(2) Université de Strasbourg, Institut Le Bel, LSAMM, 4 rue Blaise Pascal, 67070 Strasbourg, France

Hemicryptophanes are molecular cages well known for their great properties of encapsulation via non-covalent interactions, making them compounds of interest for molecular recognition, catalysis and transport of chemical species.[1] They are based on a functionalized cyclotriveratrylene (CTV), which is inherently chiral and mostly linked to a variable C_3-symmetrical moiety. An underused CTV analog is the cyclotetraveratrylene (CTTV),[2] a chiral assembly of four veratrole units that could give access to C_4-symmetrical cages. Among the C_4-symmetrical building blocks, porphyrins are highly valued for their complexation abilities, photophysical properties and have proven their efficiency in catalysis.[3]

Here, we aim to obtain new molecular cages that combine CTV/CTTV and porphyrin assets in order to perform enantioselective photocatalysis (Figure 1). For this purpose, cages based on porphyrin and CTV have been synthesized, yielding C_1-symmetrical cages. In parallel, the CTTV based analogs were also studied, paving the way to a new family of C_4-symmetrical hosts. The obtained cages will be then used for host-guest studies and enantioselective photocatalysis attempts.

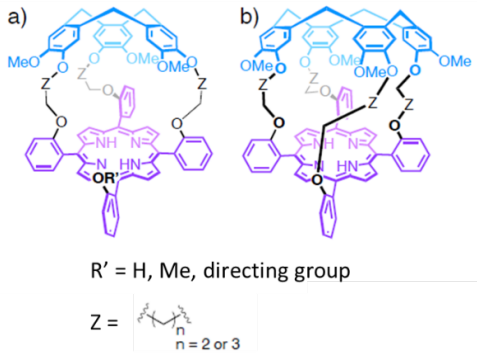

Figure 1: Targeted molecular cages based on a porphyrin and a) a CTV unit or b) a CTTV unit for an application in enantioselective photocatalysis.

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P-5

Smart-responsive alkoxyamines incorporated in silicone-based copolymers for the development of sustainable antifouling coatings

Zheng, P.(1); Thetiot-Laurent, S.(1); Joly, J-P(1); Marque, S.(1); Audran, G.(1); Matalon B.(2); Ibrahim, F.(2); Barry-Martinet, R.(2); Briand, J-F.(2); Lejars, M(2); Bressy, C.(2).

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Nowadays, maritime transportation represents over 90% of international trade and is the most used means of conveyance for the transport of goods.[1] To reduce the consumption of fuel and limit the emissions of greenhouse gases, antifouling paintings have been massively used.[2] From the tributyltin (TBT) based coatings in the mid-20th century, to the copper-based coatings often combined with biocides in the end of the 20th century,[3] these compounds were eventually all banned or heavily restricted due to their toxic effects.[4], [5] As a result, biocide-free coatings became necessary. In the 21st century, research on fluorinated polymer coatings and silicone-based paints has intensified, mainly for their low adhesion and their fouling release properties, respectively.[6], [7] Additionally, silicone-based copolymer coatings coupled with a nitroxide have shown an enhanced fouling release effect.[8]

In this context, our work aims to add an alkoxyamine in a silicone-based coating in order to combine the fouling release effect of the silicone and the rapid homolysis of alkoxyamines to form the nitroxide. To do so, we did the synthesis of 16 alkoxyamines and measured their activation energy. Their toxicity and anti-adhesion properties have also been measured by our partners in Toulon. Best alkoxyamine candidates have been selected and a methacrylate moiety has been grafted on them. The polymerization of these alkoxyamine monomers is currently under investigation in Toulon (figure 1).

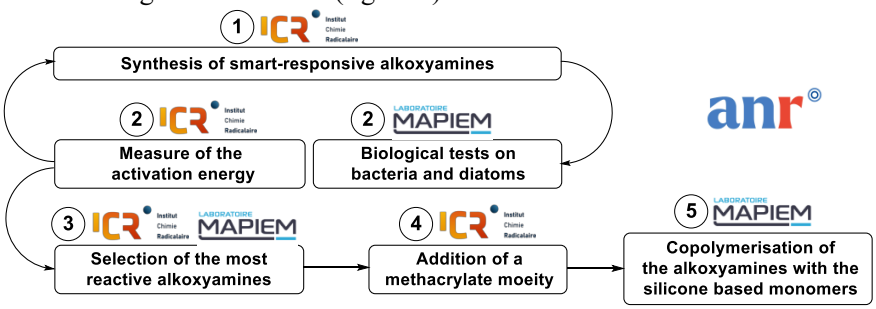

Figure 1: Overview of the current state of the project.

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P-6

An Enantioselective Gold(I)-Catalyzed Cycloisomerization of 1,6-Oxygenated Enynes toward Hedonic Derivatives

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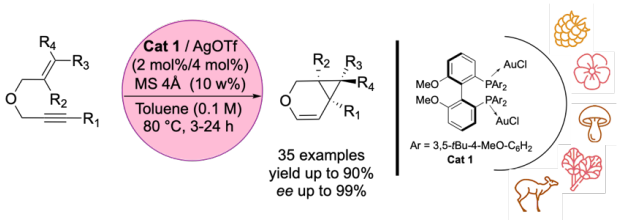
For several years, our group has focused on gold-catalyzed reactions[1,2,3] and more specifically on the gold-catalyzed cycloisomerization of 1,6-enynes in racemic conditions.[4] A novel synthetic methodology concerning the gold-catalyzed enantioselective cycloisomerization has been developed starting from readily available 1,6-oxygenated enynes precursors. The optimization of the reaction conditions allowed, in the presence of the chiral cationic Au(I) catalyst (*S*)-DTBM-MeOBIPHEP-$(AuCl)_2$ associated with AgOTf as co-catalyst, an efficient access to functionalized bicyclic adducts. Although this reaction has been studied by various groups, none has succeeded in obtaining excellent yields and excellent enantiomeric excesses for light molecules.[5,6] This efficient synthesis led to new volatile 3-oxabicyclo-[4.1.0]-hept-4-enes in excellent enantiomeric excesses ranging from 87–99%. In addition to the olfactory applications[7] of these compounds, whose odor depends on the major enantiomer, post-functionalizations have been carried out to further enhance their value.[8]



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P-7

Direct di-functionalization of ynamides mediated by visible light.

Almeida Do Amaral, L.(1); Mouysset, D.(1); Siri, D.(1); Suppo, J.-S.(1); Gastaldi, S.(1); Bertrand, M.(1); Feray, L.*(1)

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Enamides are stable electron rich double bonds that are commonly used in organic synthesis for incorporation of nitrogen functionality.[1] The stability of these units, related to their diminished enaminic reactivity, as the result of the presence of electron-withdrawing group on the nitrogen atom, is well demonstrated by their occurrence in various bioactive natural products.[2] During the course of our investigation on the reactivity of ynamides in radical chemistry, [3] we found out a strategy for accessing these powerful and versatile building blocks from ynamides in a simple, clean, and atom economical manner. The process occurs with high yield and high regio- and stereoselectivity leading to complex alkenes bearing no less than three heteroatoms.

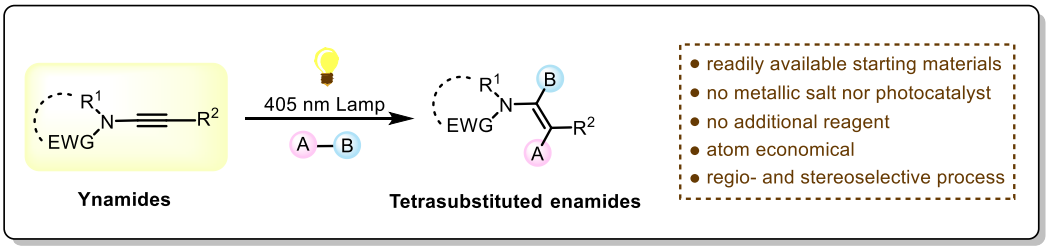

Figure 1: Tetrasubstituted enamides through direct di-functionalization of ynamides

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P-8

Towards Understanding Substituent-Controlled Excited-State Behaviour in Hemicyanine Dyes

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Hemicyanine dyes are promising photoresponsive chromophores whose optical and photochemical properties can be tuned through structural modification. In this work, a series of stilbazolium-type hemicyanine derivatives with varying substitution patterns is investigated to understand how substituent type, position, and multiplicity influence excited-state behaviour in solution. The study combines experimental NMR spectroscopy, UV-vis absorption and fluorescence spectroscopy[1,2] with time-dependent density functional theory calculations to relate spectroscopic behaviour to underlying electronic and structural features[3]. The project is focused on identifying structure-property relationships relevant to photoisomerisation and competing excited-state pathways in polar media. Particular attention is being given to the role of substitution pattern, medium effects, and the balance between electronic redistribution and geometric response following excitation. In parallel, the work also examines how the supramolecular environment may influence pathway selection and photochemical outcome[4,5]. This combined experimental and computational approach is intended to provide a broader framework for understanding substituent-controlled photoresponse in hemicyanine systems and to guide the future design of dyes with tuneable excited-state properties. Ongoing work includes extending the spectroscopic dataset, conducting medium-dependent studies, and further analysing excited-state properties to elucidate the factors governing reactivity in this class of compounds.

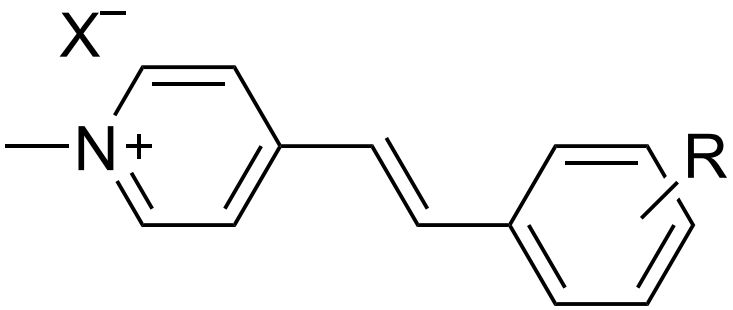

Figure 1: General structure of the quaternary hemicyanine dyes.

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P-9

Accessing 2,3-Fluoroalkynylated *N*-heterocycles *via* Gold Catalysis

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Among natural products and active compounds, nitrogen-containing heterocycles - pyrrolidines, piperidines, and azepanes - play a crucial role as core motifs.[1] To access novel candidates with improved therapeutic profiles, modifying existing structures is particularly valuable. Fluorine introduction can improve metabolic stability, lipophilicity, and bioavailability,[2] while alkynylation provides a handle for further derivatization.[3] Although these two reactions have been well-described independently, a one-step fluoroalkynylation remains under-explored and limited to aryl-alkenes substrates.[4]

In this context and following our endeavor towards gold-catalyzed access to *N*-heterocycles,[5] we embarked on the development of a gold-catalyzed fluoroalkynylation reaction applied to 2,3-unsaturated *N*-heterocycles. This transformation was optimized and was made possible by the use of Selectfluor as electrophilic fluorinated agent combined with the nucleophilic addition of a terminal alkyne activated by a gold complex.[6] This approach gave rise to the diastereoselective preparation of unprecedented 2-alkynyl-3-fluoro-*N*-heterocycles. This presentation will show the latest results on sustainable access to functionalized heterocycles.

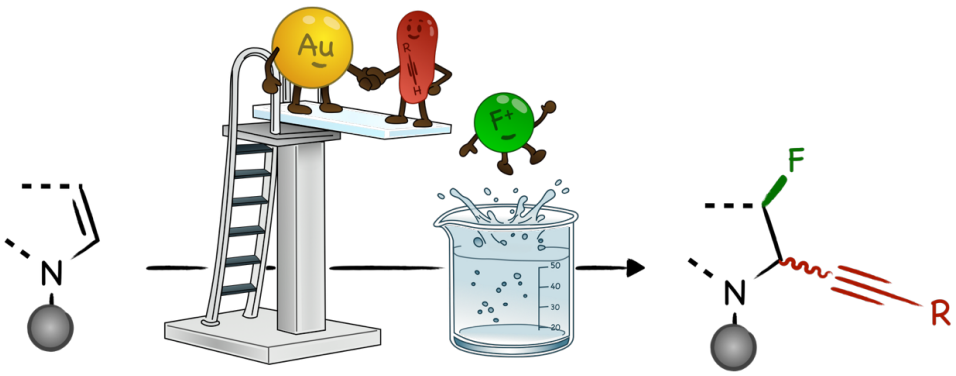

Figure 1 : Gold-catalyzed fluoroalkynylation reaction

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P-10

Efficient and stereodivergent synthesis of polyfunctionalized maleimides bearing multiple stereogenic elements

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Abstract : Chiral molecules bearing multiple stereogenic elements are common in natural and pharmaceuticals products, where stereochemistry strongly influences biological activity. [1] However, classical asymmetric catalysis methods often lead to a single major diastereoisomer. Diversity-Oriented Synthesis, particularly reagent-based approaches using chiral reagents, enables the generation of molecules with broad structural and stereochemical diversity from a common substrate. [2]

In this context, we develop a stereodivergent synthetic strategy aimed at controlling C-N axial chirality through the desymmetrization of *N*-aryl maleimides using chiral derivatives in the presence of a base. This approach provides access to polyfunctionalized maleimides bearing multiple stereogenic elements, with moderate to good yields (48-69%) and excellent stereoselectivity (ee = 95-99%).

These results demonstrate the efficiency of this methodology for the synthesis of chiral molecules featuring a C-N stereogenic axis, thereby offering new perspectives for pharmaceutical chemistry. [3]

Keywords : stereodivergent synthesis, polyfunctionalized maleimides, C-N stereogenic axis.

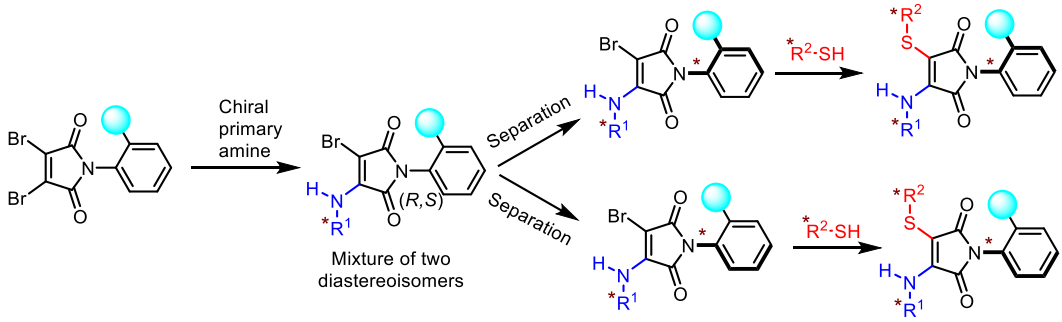

Figure: Stereodivergent synthesis of polyfunctionalized maleimides.

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P-11

A Remarkable Catalyst-Free Photochemical Alkene Hydrophosphination with Bis(trimethylsilyl)phosphonite

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Organophosphorus compounds play a central role in medicinal chemistry, catalysis, and agrochemical applications.[1],[2] Despite extensive efforts, direct alkene hydrophosphination remains challenging and often requires metal catalysts or photocatalysts, while substrate scope and functional group tolerance are frequently limited. Herein, we report a catalyst-free photochemical hydrophosphination of alkenes using bis(trimethylsilyl)phosphonite generated in situ under mild conditions.[3] Upon light irradiation, efficient P–H addition proceeds without the need for an external photocatalyst. Remarkably, the methodology extends to aromatic alkenes, overcoming limitations previously reported in related systems.[4] Mechanistic investigations suggest that photoactivation of the silylated phosphonite enables a distinct reactivity pathway, leading to highly regioselective P–C bond formation. The silylated adduct obtained after hydrophosphination constitutes a versatile synthetic intermediate. This key platform provides straightforward access to phosphinates, phosphonates, thiophosphonates, α-hydroxyphosphinic acids, and phosphinic acids. (Figure 1). Furthermore, this methodology was successfully applied to the synthesis of a pharmaceutical compound and structurally related analogues, highlighting its synthetic utility and potential for late-stage functionalization.[5],[6]

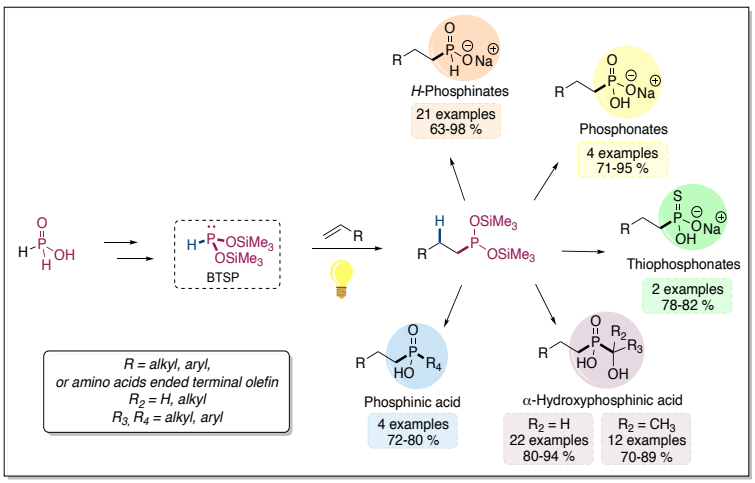

Figure 1: Hydrophosphination via a key silylated intermediate enabling access to various organophosphorus compounds

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P-12

A state-of-the-art NMR platform dedicated to research and innovation in the PACA region.

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(1) *Institut de Chimie de Nice (UMR 7272) – 28 avenue de Valrose- 0600 Nice*

The Chemistry Technology Platform (PFTC) of the Institut de Chimie de Nice is a shared facility open to both academic and industrial users. It consists of three services : Nuclear Magnetic Resonance (NMR), Mass Spectrometry (MS), and Molecular Modelling (MM).
Since December 2024, the NMR platform has been equipped with a **next-generation spectrometer, an Ascend EVO 600 MHz – AVANCE NEO with a QCI cryoprobe**. Installed for the first time in France by BRUKER, this instrument was funded through the METABOLOME project (€1.462 million). The funding results from a joint initiative involving the French State, Région Sud, Université Côte d'Azur, and the CNRS within the framework of the CPER 2021–2027 program. This instrument stands out in several respects. First, its 14.7 Tesla magnetic field provides **a 12% gain in spectral resolution** compared with a 500 MHz spectrometer, enabling improved analysis of NMR signals. Second, the system benefits from the high sensitivity of its probe, an inverse four-nucleus cryoprobe ($^{1}H/^{19}F–^{13}C$, ^{15}N, ^{31}P). Its design reduces the electronic noise associated with the NMR signal by a factor of four. As a result, **the sensitivity gain** (up to eightfold for proton detection) significantly **lowers detection limits** and reduces acquisition times. Finally, the spectrometer is equipped with several advanced accessories, including: an automated temperature regulation system (BCU II) operating from –40 °C to +70 °C, a 24-position sample changer, enabling high-throughput analysis. Thanks to this configuration, the spectrometer is particularly well suited for the study of small molecules of natural origin at trace levels or synthetic compounds, as well as biomolecules such as proteins, RNA, and DNA. The main applications include: structural analysis using 1D, 2D, and 3D NMR, characterization of ligand/biomolecule interactions, kinetic studies, metabolomics analysis, quantitative NMR.
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Figure 1: Ascend EVO 600 MHz AVANCE NEO with a QCI cryoprobe

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P-13

Gold-Catalyzed Asymmetric Cycloisomerization of *N*-Alkenylamide-1,6-enynes

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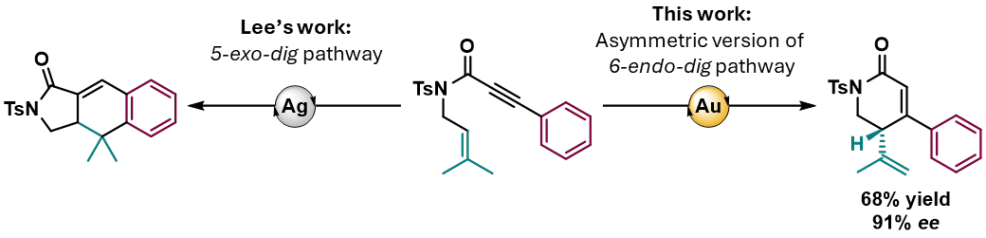
The growing use of transition-metal catalysts, particularly gold, has gained considerable attention due to their broad applicability in chemical transformations and their alignment with the principles of green chemistry [1-2]. Among various substrates, amide-1,6-enyne scaffolds have been reported to undergo cyclization via two distinct pathways – *5-exo-dig* and *6-endo-dig* – leading to different products depending on the catalytic system used [3, 4]. This study focuses on the development of an enantioselective *6-endo-dig* cycloisomerization, a reaction that remains underexplored in the literature. The optimal conditions involved the use of the chiral gold catalyst (*R*)-DTBM-MeO-BIPHEP-$(AuCl)_2$ in the presence of $AgSbF_6$ as a co-catalyst in toluene at 40 °C. Under these conditions, the *6-endo-dig* cyclized products were obtained in good yields (**50-68%**) with excellent enantioselectivities, reaching *ee* values of **82-91%**. DFT calculations provided further insight into the divergent selectivity of silver and gold catalysts in the cycloisomerization of amide-1,6-enynes. While silver intermediates clearly favored the *5-exo-dig* pathway, gold catalysts promoted the more favorable *6-endo-dig* route.



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P-14

Expanding Multicomponent Reaction Chemistry through Graphene Oxide Carbocatalysis

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Multicomponent reactions (MCRs) represent a powerful strategy in modern organic synthesis, enabling the rapid construction of structurally diverse and highly functionalized molecular frameworks from simple starting materials. Their intrinsic advantages, including high atom economy, operational simplicity, and suitability for diversity-oriented synthesis (DOS), make MCRs particularly attractive for the efficient generation of molecular complexity[1].
In this context, carbocatalysis has emerged as a versatile and sustainable catalytic platform, with graphene oxide (GO) being one of the most widely used carbon-based carbocatalysts in organic synthesis. In multicomponent reaction chemistry, carbon-based catalysts can operate in two conceptually distinct ways: they can directly promote the formation of target molecules, enabling structural diversification[2], or generate highly reactive intermediates in situ, such as imines formed through C–N bond oxidation, which can then be intercepted in multicomponent reaction manifolds. In the latter case, the carbocatalyst plays a key role in the controlled generation of reactive species involved in oxidative multicomponent assembly.
Building on these complementary roles, our research explores the integration of carbocatalysis with multicomponent reaction design under both thermal and photochemical activation conditions. This dual approach aims to expand the reactivity landscape of carbocatalyzed processes and to enable new pathways for the efficient construction of structurally complex and functionally rich molecular architectures.

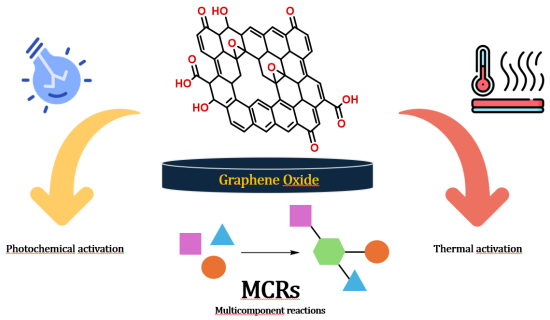

Figure 1 : MCRs promoted by Graphene Oxide

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P-15

Multicomponent Reactions Enabled by Visible-Light Activation of Renewable Cinnamoyl Diazoketones

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Motivated by our ongoing interest in isocyanide chemistry and photochemical transformations, we continue to explore light-mediated multicomponent reactions (MCRs) as sustainable synthetic strategies. In particular, we investigate the K-3CR and SK-3CR processes, originally discovered in our laboratory[1,2], in which ketenes—generated through the photochemical Wolff rearrangement of diazoketones—react with isocyanides and, respectively, with carboxylic acids or silanols to afford α-acyloxy- and α-silyloxyacrylamides. Previous studies demonstrated that replacing UV irradiation with blue light significantly improves both selectivity and efficiency.[3] In this work, we further optimize the system, aiming to extend photoactivation toward the green region of the visible spectrum while using renewable carbon-derived starting materials. In this context, the project contributes to a wider research line dedicated to the valorization of ferulic and cinnamic acid derivatives. The presence of an additional double bond in these structures is particularly attractive, not only because it may impart distinctive photochemical reactivity, but also because the resulting extended conjugation can shift absorption toward longer wavelengths, potentially enabling activation under green light.

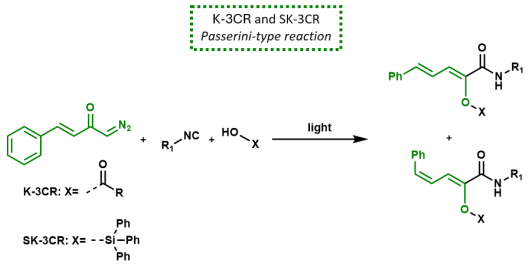

Figure 1 : Ketene three-component reaction (K-3CR) and the silylative ketene three-component reaction (SK-3CR) applied to cinnamoyl diazoketone.

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Sustainable Self-Healing Thermosetting Polymers from Renewable Carvone-Derived Diepoxides

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With the growing severity of global environmental issues and the depletion of fossil resources, the demand for clean fuels and green chemicals is rapidly increasing.[1] Monoterpenes represent a versatile class of renewable molecules, some of which possess promising potential as monomers for polymer synthesis.[2,3] In this study, carvone[4,5] was utilized as a renewable precursor to synthesize and oxidize a series of diepoxide derivatives, which were subsequently cured with glutaric anhydride in the presence of imidazole to obtain four fully bio-based thermosets.[6] Mechanical testing revealed that the hydroxyl-functionalized thermoset exhibited the best overall performance and, notably, demonstrated excellent self-healing ability without the need for additional catalysts. This work provides a sustainable route for developing renewable, self-healing epoxy thermosets derived from natural terpenes.

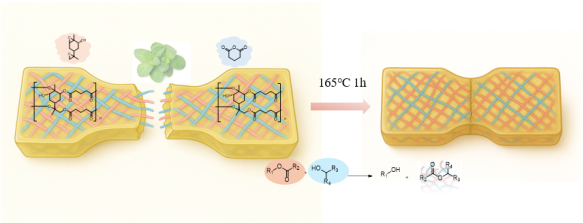

Figure 1: Thermal self-healing behavior of the carvone-derived polymer network at 165°C for 1 h

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P-17

Alkoxyamine synthesis from carboxylic acid using reductive photoredox cycle

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The formation of carbon-oxygen bonds is a key reaction in organic synthesis that has been widely described in the literature, as it allows for the production of numerous functional groups, including alcohols, ethers, esters, acids, phenols, and carbonyls, which are found everywhere: pharmaceuticals, natural products, polymers, perfumes, and fuels. Among functional groups containing a C-O bond, alkoxyamines are versatile moieties that can serve both as precursors for various functional groups and as reactive sites since they behave as excellent radical reservoirs. Although the formation of alkoxyamines by radical trapping has been regularly reported, many examples focus primarily on providing evidence for radical mechanisms rather than on the synthetic efficiency of this reaction. Recent studies highlight the use of photocatalytic oxidative or reductive cycles to achieve this transformation.[1,2]
Currently, our research focuses on trapping carbon-centered radicals using various starting materials in the presence of nitroxides to generate the corresponding alkoxyamines. Starting from simple carboxylic acids, the reaction proceeds under mild conditions through a photocatalytic decarboxylation process. The resulting carbon-centered radical is then trapped by a nitroxide to yield the corresponding alkoxyamine. This transformation takes place within a photocatalytic reductive cycle. Such an approach offers a sustainable and versatile method for constructing of alkoxyamines from readily available substrates.

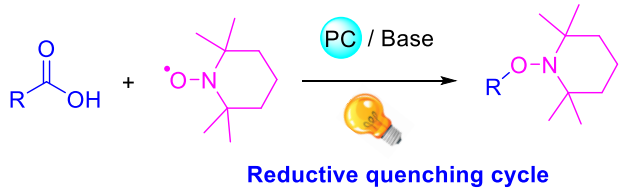

Figure 1 : Alkoxyamine synthesis using reductive quenching cycle

The scope and limitations of the reaction, as well as the study of the influence of the structure of the substrate on the efficiency and selectivity of the radical trapping process will be discussed.

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P-18

New chlorinated steroids from the marine sponge *Coelosphaera* sp.

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Marine sponges are prolific sources of unique secondary metabolites, with approximately 200 new compounds isolated annually, many exhibiting potential biological activity [1]. While many sponge genera have been extensively studied, the chemical constituents of genus *Coelosphaera* remain entirely unexplored. Herein, we report the first chemical investigation of a *Coelosphaera* sp. specimen collected in the Marquesas Islands (Nuku Hiva, Pointe Matateteiko), French Polynesia.

Preliminary UHPLC–HRMS/MS analysis and dereplication of the sponge crude organic extract revealed the presence of several polyoxygenated sterols and rare chlorinated steroid derivatives. Subsequent fractionation by silica gel column chromatography, followed by purification using HPLC, led to the isolation of nine steroidal metabolites, including five previously undescribed steroid derivatives, along with the previously reported chabrolosteroid E and kiheisterones C–E. Their structures were elucidated using extensive HRMS and 1D and 2D NMR spectroscopic data.

Our investigation of the genus *Coelosphaera* reveals its first-ever reported chemical profile, characterized by a diverse array of non-chlorinated sterols and novel chlorinated steroid analogues. These findings expand our knowledge of the structural diversity of chlorinated steroids, which are rarely reported in marine sponges. Given the diverse bioactivities of steroids such as anticancer, antimicrobial, and anti-inflammatory properties [2], these new metabolites are scheduled for pharmacological evaluation to determine their therapeutic potential. This work highlights the untapped chemical diversity of rare marine sponges and provides new insights into halogenated sterol biosynthetic pathways.

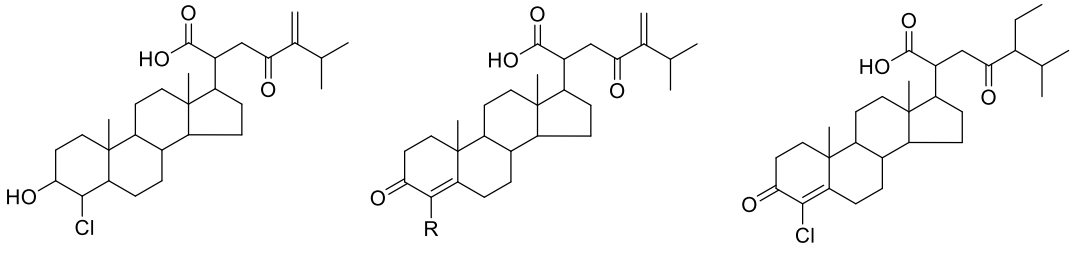

Figure 1: The chemical structure of known isolated steroids

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[2] Bioorg. Chem., 2024, 153, 107933.

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Development of new triazoles triggering apoptosis and ferroptosis for leukemia treatment

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Acute leukemias represent one of the most common malignant disorders. Recently, targeted therapies made real breakthroughs in Chronic Myeloid Leukemia (CML) and Acute Myeloid Leukemia (AML) treatments, drastically improving survival rates.[1,2] Most of the drugs used in these targeted therapies are tyrosine kinases inhibitors (TKIs) targeting BCR-ABL or FLT3) and IDH or BCL-2 inhibitors. These drugs mainly induce cell death through apoptosis and are subject to resistance, thus limiting their efficacy.[1,3] Recent studies highlighted ferroptosis as a promising strategy to cause cell death. Our work focuses on the development of new inhibitors that trigger AML cell death through both apoptosis and ferroptosis, aiming to overcome therapeutic resistance.[4] Two compounds, a nucleoside (231) and a non-nucleoside analogue (HA344), have shown strong activity against CML K562-S cells (Figure 1). We recently identified GPX4 and TXNRD1 as targets through a click chemistry approach coupled to mass spectrometry.[4] Despite strong *in vitro* activity, these compounds suffer from short half-life *in vivo* due to fast ester hydrolysis. Consequently, our recent work focuses on replacing these ester moieties to improve *in vivo* stability. Additionally, we are pursuing a Structure-Activity Relationship (SAR) study, designing new analogues, to improve GPX4 and TXNRD1 inhibition.

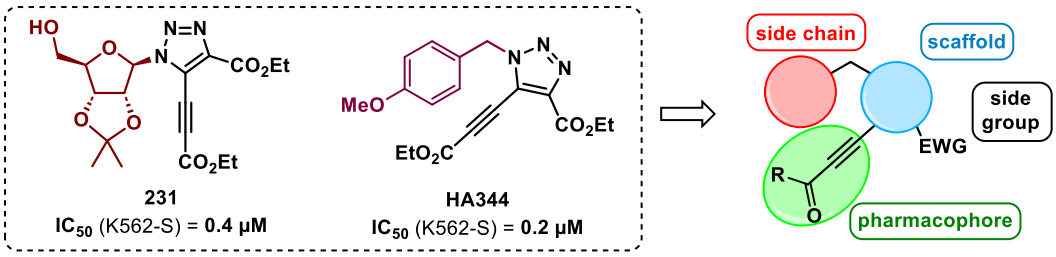

Figure 1. Structure, activity and SAR map of triazole analogues 231 and HA344

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P-20

Transition metal-free alkynylation of enaminomaleimides with α-chloronitroolefins- Syntheses of new functionalized maleimides

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Maleimides, or 1*H*-pyrrole-2,5-diones, represent a key electrophilic heterocyclic motif in organic chemistry. Over the past century, this five-membered heterocyclic imide core has been identified in diverse families of natural products,[1] synthetic pharmaceutical molecules,[2] and functional polymers,[3] offering broad scientific and technological applications. These maleimides are recognized for their C=C double bond conjugated to two carbonyl groups, which confers electrophilic properties enabling Michael addition reactions (particularly with thiols) and Diels–Alder cycloadditions with dienes. However, their (pro)nucleophilic characteristics remain poorly characterized in the literature and largely unexplored. A method to probe their nucleophilicity is the utilization of enaminomaleimides, or α-aminomaleimides.[4] They are a subclass of maleimide derivatives in which an amino group is introduced at the α-position (or position C3). During our research aimed at exploring the nucleophilic potential of enaminomaleimides, we serendipitously uncovered a particular reactivity of these species with α-chloronitroolefins. Instead of yielding the anticipated maleimide-fused pyrroles,[5] the reaction resulted in an alkynylation at the C4 position of the enaminomaleimides. Notably, in contrast to conventional alkynylation protocols, this approach successfully avoids the use of transition metals. Furthermore, this reaction exhibits a broad substrate scope, proceeding smoothly with a variety of α-chloronitroolefins and enaminomaleimides to afford the corresponding products in excellent yields (up to 93%). Conducted under mild and operationally simple conditions, this unique reactivity opens a novel synthetic pathway in enaminomaleimide chemistry and offers extensive possibilities for further functionalization.

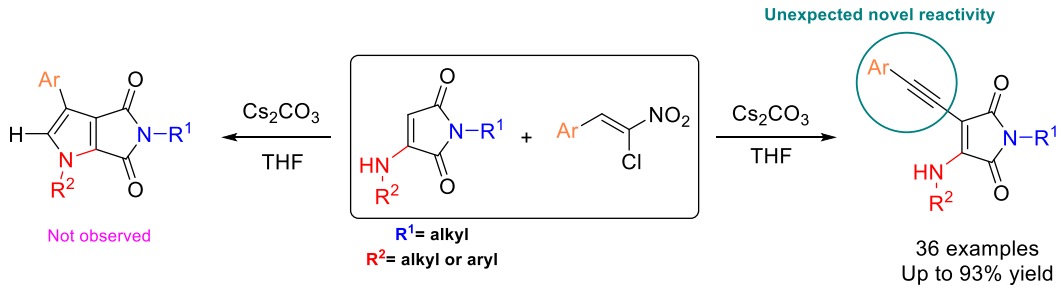

Figure 1: Unprecedented reactivity of enaminomaleimides with α-chloronitroolefins under basic conditions

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Synthesis and characterization of biodegradable cellulose-based films for food storage: challenges and perspectives

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Food packaging plays a key role in protecting and preserving food; however, the extensive use of non-biodegradable synthetic plastics has raised significant environmental concerns. In this context, the development of biodegradable and sustainable materials based on biopolymers represents a hot topic of scientific research in a circular economy perspective[1]. Within this framework, we exploited soybean hull-derived cellulose, modified into carboxymethyl cellulose (CMC)[2], for films' preparation, trying several compositions.
To improve their performances, grape pomace-derived polyphenols have also been incorporated into the best formulation. The resulting samples have been deeply characterized and their bioactivity and biodegradability have been tested as well. The developed films showed good mechanical properties, antioxidant activity and biodegradability, confirming their potential for sustainable food packaging; however, further studies on permeability and different food types are needed to fully evaluate their functional and protective efficacy.

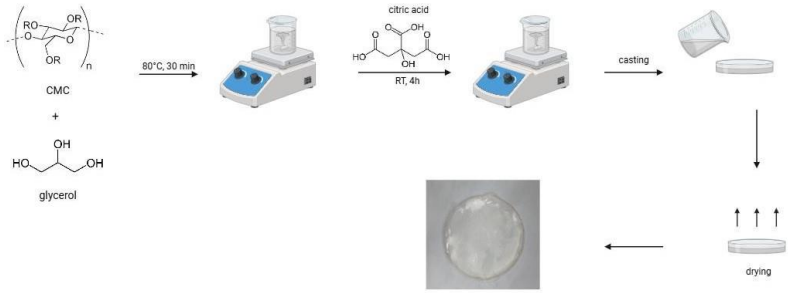

Figure 1 : Films preparation scheme

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A new insight into the sources of particulate matter reaching the East Antarctic plateau by lead isotopic analysis

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Particulate matter (PM), emitted by both natural and anthropogenic sources, plays a key role in global climate regulation and in the long-range transport of pollutants. When these particles are formed, they can travel for long distance, reaching the most isolated regions on Earth, like Antarctica. A complete characterisation of sources, transport and composition of PM reaching this pristine region is necessary in order to monitor the global impact of human activities [1]. This study, connected to the project SIDDARTA ("Source identification of (mineral) dust to Antarctica") of the Italian National Antarctic Research Program, aims at identifying the natural and anthropogenic sources of PM reaching inland Antarctica. To reach this purpose, PM_{10} samples from 2017 to 2024 have been collected from Dome C, in the East Antarctic plateau. In addition, to evaluate the impact of potential source areas (PSA), soil samples from Australia and Patagonia have been also collected. To achieve a reliable comparison with the composition of PM reaching Antarctica, soil samples have been resuspended using a home-made resuspend chamber and the $PM_{2.5}$ resulted has been collected onto PTFE filters [2]. The lead isotopic composition of these samples has been determined using inductively coupled plasma mass spectrometry (ICP-MS), which enabled the identification of their provenance. Comparing the isotopic composition of PSA and PM_{10} samples made it possible to highlight a mixed contribution of Patagonia and Australia sources to Antarctic PM.

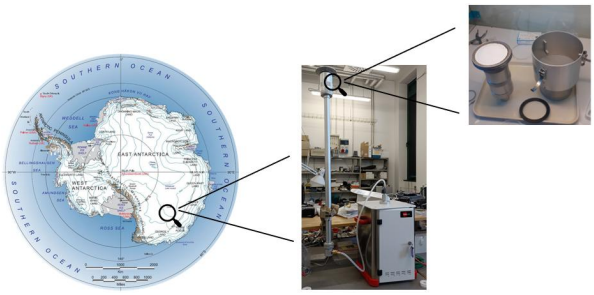

Figure 1: PM_{10} sampling at Dome C (Concordia Station): sampling device.

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P-23

Optimized MicrowaveDriven- Michael Addition for the Synthesis of Levoglucosenone--Derived Amphiphilic Molecules

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A rapid, safe, and sustainable procedure was developed for the synthesis of a library of amphiphilic molecules derived from levoglucosenone (LGO), in alignment with the objectives of the EU Chemicals Strategy for Sustainability. LGO, a biobased building block obtained from cellulose-rich nonedible biomass, offers a versatile platform for the development of high value derivatives. The amphiphilic nature of the adducts prepared in this work highlights the potential for generating surfactant-like structures entirely from lignocellulosic feedstocks—an attractive prospect considering that, in Europe, renewable surfactant production still relies predominantly on oleochemical sources such as vegetable oils.[1] LGO was employed in a microwave-assisted Michael addition using a series of alkyl malonates (dimethyl, diethyl, dibutyl, and dibenzyl) to afford structurally diverse products. The intrinsic miscibility of the reagents enabled solventless conditions, while the use of an inexpensive, nontoxic inorganic catalyst, $Ca(OH)_2$, ensured high selectivity toward the desired adducts. Reaction conditions were optimized through a multivariate Design of Experiments (D-optimal) approach, yielding reproducible gravimetric yields above 80%. Diastereoselectivity was confirmed by X-ray crystallographic analysis of the simplest LGO derived diester. The physical properties of the four synthesized adducts were investigated using an integrated set of experimental and theoretical methods, including Hydrophilic–Lipophilic Balance calculations, COSMO-RS simulations, octanol/water partition coefficients, contact angle measurements, and emulsion tests. These results collectively reveal the promising potential of these LGO-based compounds as future surfactant candidates derived from lignocellulosic biomass.[2,3]

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P-24

One-pot synthesis of MOFs from PET waste

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Plastic waste and water pollution demand circular economy-driven innovations. Polyethylene terephthalate (PET) is one of the most widely used synthetic polymers (e.g., in beverage packaging, textile manufacturing, and electronic devices), and its improper disposal causes severe environmental harm. [1] Depolymerized PET yields terephthalic acid and ethylene glycol—essential precursors for the synthesis of metal-organic frameworks (MOFs), versatile porous materials widely studied for their applications in gas storage, separation, and catalysis. [2]
The synthesis of MOFs from PET waste can be achieved either through a two-step process involving depolymerization of PET followed by MOF synthesis, or through a single-step process, where depolymerization and MOF formation occur simultaneously. [3]
In this study, we investigate the direct synthesis of MIL-101(Cr) and MIL-53(Al) starting from PET waste, under hydrothermal conditions. The obtained products were structurally characterized by PXRD, FT-IR, and Raman spectroscopies. Their morphology and particle size were investigated by FESEM, and the specific surface area was determined.
Results indicate that the obtained products are analogous to those synthesized with commercial terephthalic acid in term of crystallinity, but present different morphology and surface area.
This approach not only addresses plastic pollution but also offers a more sustainable and cost-competitive pathway for MOF synthesis.

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P-25

Sustainable synthesis of hydroxyapatite-containing composites from eggshells for soil amendment applications

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Managing large volumes of food waste is a growing challenge. Eggshells (ESs) are an abundant and widespread waste that represent an interesting source for Ca-based materials.[1] To fulfil the cradle-to-cradle sustainability concept, the final products need to be materials that can either degrade or serve as nutrients in soil. ES can be converted into different Ca precursors to obtain hydroxyapatite (Hap) nanoparticles, a promising solid fertilizer that can promote a controlled release of nutrients.[2] Most of the reported procedures involve a high-temperature calcination step to obtain CaO, a process that is energy-intensive and CO_2 emitting.[3]
This study explores a sustainable approach by dissolving ES in an ascorbic acid solution, a green, non-toxic, and cost-effective reagent. The synthesis was performed using a wet chemical precipitation method.
Composition, crystallinity and morphology of the obtained product were compared to those of Hap obtained with commercial reagents and by dissolving ES in nitric acid.
Nutrient release behaviour was evaluated through ICP-OES, demonstrating the material's potential for agricultural applications. This method offers a low-impact, circular approach to waste valorisation, promoting the conversion of food waste into high-value functional materials.

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Toward greener agriculture: chemical profiling and environmental fate of a plant-derived biostimulant

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The widespread use of synthetic pesticides and fertilizers to increase crop production has raised concerns due to their persistence in the environment and potential accumulation in the food chain, leading to negative ecological and human health effects [1]. To avoid this, plant-derived biostimulants are increasingly proposed as eco-compatible alternatives to enhance crop performance while reducing environmental burden [2]. However, robust evaluation of their chemical composition and environmental behaviour is essential to ensure both efficacy and sustainability. Within this scenario, a novel plant-derived biostimulant was characterized to fully unravel its composition and environmental fate in a representative Thai soil to assess both its potential and possible drawbacks.
Elemental composition was assessed by ICP-MS, while LC-HRMS and GC-MS analyses enabled detailed profiling of the main organic constituents, comprising the more volatile fraction. The product exhibited high phenolic content and antioxidant capacity, supporting its potential role in plant stress mitigation. Regarding the environmental distribution experiments, soil characterization revealed a kaolinite-rich matrix with limited adsorption sites and low permeability. Batch adsorption experiments demonstrated rapid retention of selected marker components, with more than 80% adsorption within 30 minutes and equilibrium reached within 16–24 hours. Adsorption data were best described by a Langmuir isotherm, indicating strong and relatively uniform surface interactions. The preferential retention of the biostimulant in surface soil layers suggests limited leaching potential and reduced risk of groundwater contamination. Combined with its plant-derived origin and bioactive properties, these findings support the potential of this formulation as a more sustainable agricultural input. Overall, this work provided an integrated chemical and environmental assessment, contributing to the development of safer and environmentally responsible crop management strategies.

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A sunlight-compatible photochemical thiol-ene reaction promoted by *para*cyclophane-derived photocatalyst

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Photosensitizers are light-sensitive molecules that can generate reactive species such as radicals, cations, or anions, upon excitation by a light stimulus. Light-induced processes continue to evolve rapidly and are increasingly integrated into industrial applications. Nowadays, the development of high-performance photosensitizers that are efficient, environmentally friendly, non-toxic, and responsive to visible light is a major research focus. Most conventional photosensitizers are highly sensitive to UV light.[1] Consequently, the limited number of visible-light photosensitizers highlights the need for the development of new structures specifically designed to exhibit controlled reactivity.

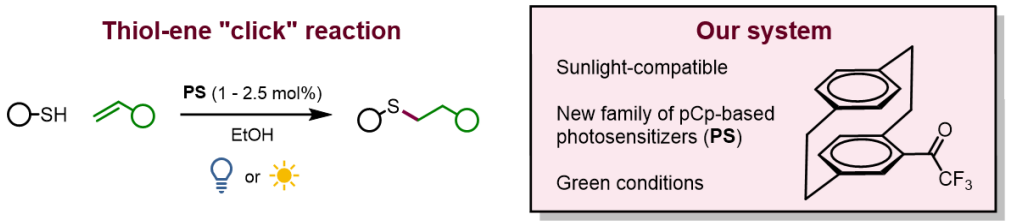

Figure 1: Thiol-ene "click" reaction using [2.2]paracyclophane derivative as photosensitizer

In our research, we focused on the design of novel photosensitizers by using the unique properties of [2.2]paracyclophane frameworks. Recent advances in radical chemistry have demonstrated that through-space electron delocalization within such scaffolds can significantly enhance the stability of carbon-centered radicals.[2] Building on this concept, we synthesized a trifluoromethylketone-substituted [2.2]paracyclophane derivative. This molecule exhibits absorption in the visible region, specifically at 405 nm. This new compound acts as an efficient photocatalyst for thiol-ene "click" reaction under green conditions, including the use of green solvent, low catalyst loading, ambient temperature and sun-light compatible.[3]

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Speciation and transfert mechanisms of actinides in marine phytoplankton

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Seawater constitutes both the final sink and the largest reservoir for contaminated waters, making it a key environmental compartment for monitoring radioactive metal contamination. Among these elements, actinides of natural or anthropogenic origin represent major radiotoxic pollutants whose bioaccumulation and transfer within marine ecosystems raise significant environmental concerns. [1]

Phytoplankton is a particularly relevant model for studying the entry of these elements into the food chain. Located at the base of the marine trophic web, it can accumulate these contaminants and may therefore influence their transfer to higher trophic levels. Among the actinides present in the environment, plutonium-239 is of particular interest: it serves as a tracer of fallout from nuclear weapons testing and is among the most radiotoxic elements. [1] Understanding its behavior in the marine environment is therefore essential. However, experimental studies remain limited due to its high radiotoxicity and the constraints associated with its handling, making the use of more easily manageable chemical analogues necessary.

In this context, thorium-232 was selected as a chemical analogue of plutonium. Two representative forms were investigated: a molecular complex, $Th(NTA)_2$, and colloidal nanoparticles of ThO_2. The different thorium species were characterized and quantified using ICP-MS, BET, TEM, and XRD, following optimization of synthesis and mineralization methods. Initial experiments enabled the development of a mineralization method compatible with the sorption behavior of thorium. TEM observations, conducted to characterize and monitor particle aging in seawater, revealed a strong tendency for ThO_2 nanoparticles to aggregate in this medium.

These results represent a first step toward understanding the physicochemical behavior of the studied systems in seawater. In a second step, they will enable the evaluation of their accumulation potential in the marine phytoplankton *T.Isochrysis Galbana*, with the aim of investigating plutonium chemical speciation at the molecular scale in this species of interest.

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Role of iron and other trace elements in controlling biological activities and biogeochemical cycles in the Ross Sea (Antarctica)

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Primary productivity in large areas of the Southern Ocean is limited by the availability of dissolved iron, an essential element for phytoplankton metabolism. [1]
A better understanding of the iron partitioning is needed to predict changes in Fe availability in the future ocean. In fact, climate driven changes in the productivity of phytoplankton and microbial communities will impact the Ross Sea Fe biogeochemistry, by modifying the balance among biological uptake, chemical speciation, vertical export and organic matter recycling. [2]
This work analyzes the distribution of iron and other bioactive trace elements through an integrated study of the dissolved and particulate fractions (i.e. retained by a 0.20 µm pore size polycarbonate filter) with the aim of broadening the interpretation of the biogeochemical processes taking place in the Ross Sea.
Sea water samples were collected on board of R/V Laura Bassi in the framework of the IBIZA project (**I**ron-**B**inding organic ligands – planktonic microbes **I**nteractions in coastal and offshore **Z**ones of the Ross Sea, **A**ntarctica) activities during the XL Italian expedition of the "Programma Nazionale di Ricerche in Antartide" carried out in the 2024-25 austral summer.
Dissolved elements were determined by ICP-DRC-MS (Inductively Coupled Plasma Mass Spectrometer with Dynamic Reaction Cell), following a coprecipitation procedure with $Mg(OH)_2$. Particulate elements were determined by ICP-AES (Inductively Coupled Plasma Atomic Emission Spectrometer) after a microwave assisted acid digestion of the suspended particulate matter.
The analytical methods were validated through procedural blanks, detection limit evaluation, and the use of certified reference materials to ensure data accuracy and reliability. The results revealed significant spatial and vertical variability of trace metals, influenced by water mass characteristics and biological processes. The use of Principal Component Analysis, in which chemical data were considered together with the main environmental and biological parameters, allowed to identify some factors controlling the variability of the system in surface and subsurface samples, where biological assimilation can play a decisive role in conditioning the distribution of trace metals.

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Solvent-Free Dehydrogenation of Alcohol-Based Liquid Organic Hydrogen Carriers through Catalytic Acceptorless Coupling: from Bench Scale towards Kilo Scale

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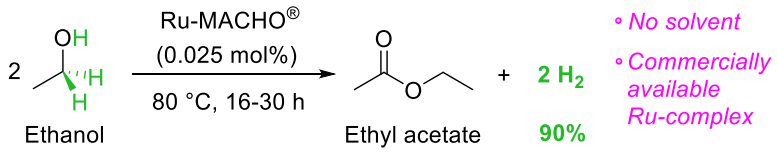
Homogeneous catalytic dehydrogenation (DHY) of suitable and easily achievable organic compounds plays a key role in the transition towards a sustainable hydrogen economy. In this context, Liquid Organic Hydrogen Carriers (LOHCs) are particularly attractive due to their favorable hydrogen storage capacity (4–12 wt%) and their ability to be handled as liquids under operational conditions, facilitating solvent-free processes.[1] While industrial research has mainly been focused on aromatic systems such as dibenzyl toluene, able to store up to 6.2 wt% of H_2, these require harsh reaction conditions (200–250 °C) and originate from fossil fuel reserves. In contrast, alcohol-based LOHCs offer a safer, more sustainable alternative, characterized by higher reactivity and significantly milder operating temperatures (80–150 °C).

Herein, we report the acceptorless catalytic DHY of ethanol, 1,4-butanediol and their mixtures with ethylene glycol, using the commercially available Ru-MACHO® complex.[2],[3] These specific LOHCs were selected for their low toxicity, high availability, and cost-effectiveness.



Scheme 1: Ru-catalyzed DHY of alcohol-based LOHCs.

In a solvent-free system at 80 °C, using 1.3 mol% of sodium ethoxide as a base, ethanol gave the best outcomes, achieving ethyl acetate and a hydrogen release (measured in a continuous fashion) of 3.93 wt% (90% of the theoretical 4.38 wt% capacity) within 30 hours. These promising bench-scale results paved the way for process scale-up. Preliminary data obtained using a 4 L reactor, equipped with precise temperature and pressure controls for liquid-phase operation, demonstrated the feasibility of the process at a larger scale, marking a significant step towards the practical implementation of alcohol-based hydrogen storage.

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Iso-Oriented Aggregates of $CoFe_2O_4$ with Tunable Magnetic Properties

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Recent progress in nanostructured materials has highlighted the importance of understanding the physicochemical mechanisms governing the hierarchical assembly of nanocrystals into superstructures[1], which are crucial for the rational design of multifunctional nanomaterials. In particular, the controlled organization of magnetic nanocrystals into ordered architectures enables the combination of collective magnetic behavior with high surface area and porosity, opening opportunities for advanced applications[2].
Here, we investigate mesoporous spherical aggregates composed of ~7 nm cobalt spinel ferrite nanocrystals ($CoFe_2O_4$), that assemble into ~50–60 nm mesoporous iso-oriented magnetic aggregates with high surface areas (~120 m^2/g). Morpho-structural properties were characterized via X-ray diffraction (XRD), transmission electron microscopy (TEM) and N_2-physisorption, confirming the formation of highly crystalline nanocrystals organized into well-defined spherical mesoporous superstructures.
The cobalt content was systematically varied (Co^{2+}: 100, 75, 50 and 25%) in order to investigate its influence on the magnetic anisotropy of the system. Magnetic measurements reveal a quasi-superparamagnetic behavior at 300 K with a saturation magnetization (Ms) of approximately 80 A m^2 Kg^{-1}. At 5 K, a decrease in Ms and a corresponding increase in coercivity (Hc) are observed with decreasing cobalt content, indicating a modulation of magnetic anisotropy.
In addition, Mössbauer spectroscopy was employed to gain deeper insight into the local iron environments and cation distribution within the spinel structure. The combination of hierarchical structure, high surface area, and tunable magnetic properties makes these iso-oriented aggregates promising candidates for applications in targeted drug delivery, magnetic separation, and sensing technologies.

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Recyclability Enhancement of Siliconized Papers

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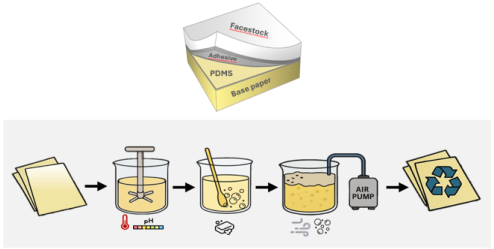
Release liners are essential components in the pressure sensitive adhesive industry, as they serve the purpose of protecting labels before their application and facilitate their dispensing. This protective layer is usually composed of smooth, lightweight yet dense and semi-transparent paper, with good barrier and moisture resistance, called glassine paper[1]. The release properties are provided by a thin layer (~ 1µm) of polydimethylsiloxane (PDMS), as the high flexibility of its chains allow for low surface energy and low energy dissipation upon peeling, resulting in low release forces[2].

However, once the label has been dispensed, the liner has ended its purpose and must be discared. The detachment and removal of the PDSM from the cellulosic fibers present several difficulties in conventional recycling mills, leading to equipment contamination and reduced fiber recovery yields. As a result, most post-consumer release liners are currently incinerated or landfilled, with only limited downcycling alternatives available. Considering the large volumes generated annually in Europe, this disposal model represents a substantial loss of valuable fibrous resources and contradicts circular economy principles[3].

In this work, a procedure for removing the silicone coating from glassine paper is proposed, enabling the recovery of fibers and promoting closed-loop recycling of siliconized release liners. Commercial siliconized paper (50g) is disintegrated under controlled thermal and alkaline conditions (70 °C, pH 10) using a hydropulping process. The resulting pulp is treated with 0.2–1 wt.% anionic surfactants to promote the detachment of hydrophobic silicone residues, followed by a flotation step to separate silicone-rich particles from the fibers. The cleaned pulp is then used to produce handsheets for characterization (Fig.1). FTIR, XRF and EDS-SEM analyses are used to study the chemical composition, morphology and residual PDMS content, while the thermal and stability and strength properties of the samples are investigated using thermogravimetric analysis (TGA) and mechanical testing. To evaluate the feasibility of reusing the recovered fibers as release liners, samples are prepared with different amounts of the recycled pulp, and the obtained handsheets are calandered and siliconized to measure their release forces.

Once the parameters are optimized to maximize fiber recovery and to maintain a good fiber quality, the scalability of this process will be assessed to evaluate its feasibility for industrial scale. With this approach, a close-loop recycling process could be applied to reintroduce desiliconized recycled fibers into new glassine production.



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Synthesis, flux growth and structural investigation of the $R_2Pd_3Si_5$ series (R = rare earth elements)

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Intermetallic compounds (IMCs) represent an interesting class of materials, as many of them are widely used for their unique physical properties, playing an important role in technological innovation. This class of materials includes the $R_2M_3X_5$ family of polar IMCs (R: rare earth and actinide elements; M: transition metal; X: p-block element)[1] which exhibits a remarkable compositional and structural variety, with more than 200 known compounds crystallizing in six different structure types. This work focuses on the $R_2Pd_3Si_5$ series aiming to investigate the stability, formation and structural behaviour of its representatives. Samples were synthesized using conventional methods, such as arc- and induction-melting, as well as the non-reactive metal flux technique[2]. The latter employs a low-melting metal solvent (Sn) to promote the synthesis or the recrystallization of IMCs and proved crucial for obtaining large and high-quality single crystals of the target phase. Therefore, a simplified and reliable characterization by scanning electron microscopy equipped with energy dispersive X-ray spectroscopy (SEM-EDXS), powder (XRPD) and single-crystal X-ray diffraction (SCXRD) was enabled. The $R_2Pd_3Si_5$ is observed for R = La, Ce, crystallizing with the *oI*40-$U_2Co_3Si_5$ structure, in agreement with literature data. In contrast, phases comprising R = Nd, Sm, Gd, crystallize as *mP*20-$Nd_2Pd_3Si_5$, representing a new prototype (Figure 1). Interestingly, $Pr_2Pd_3Si_5$ can adopt either structure type, depending on the synthesis method employed.

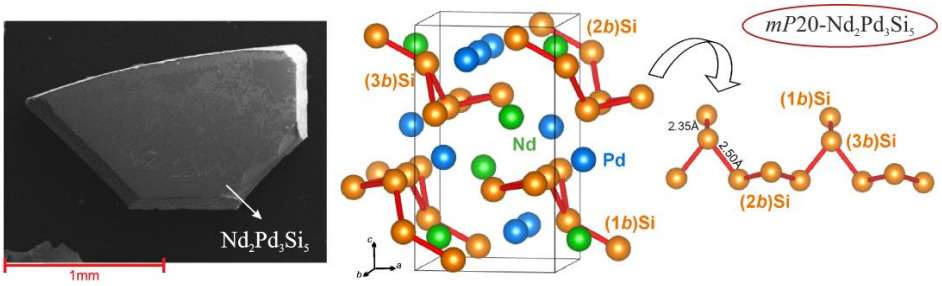

Figure 1 : SEM micrograph (left) and crystal structure representation (right) of monoclinic $Nd_2Pd_3Si_5$. Si–Si contacts at distances compatible with covalent interactions are indicated by red sticks.

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New Biosourced Thermoplastic Polymers for Composites and their Recycling by Depolymerisation

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In 50 years, the global plastic production has increased by more than 4000%, engendering various environmental issues. Yet, despite mounting evidence of detrimental environmental impact and public concern regarding both their production with fossil resources and the end of life of polymeric materials, the current approaches developed by our societies are overtaken by this ever-growing production of polymers. This project focuses on the development of new biosourced and recyclable thermoplastics for an application in composite.
Moreover, plastic recycling remains a major challenge: in Europe, only 32.5% of plastic waste is recycled, while the remainder is incinerated or landfilled. To address this issue, the project proposes an innovative depolymerization process based on the use of NIR LEDs and NIR dyes, enabling targeted polymer degradation at low temperature. Unlike current thermal methods, which are highly energy-intensive, this technology reduces energy consumption by generating heat directly within the material, thereby avoiding thermal losses.
This innovative approach is fully aligned with environmental objectives aimed at reducing the carbon footprint of plastic materials while promoting improved waste valorization.

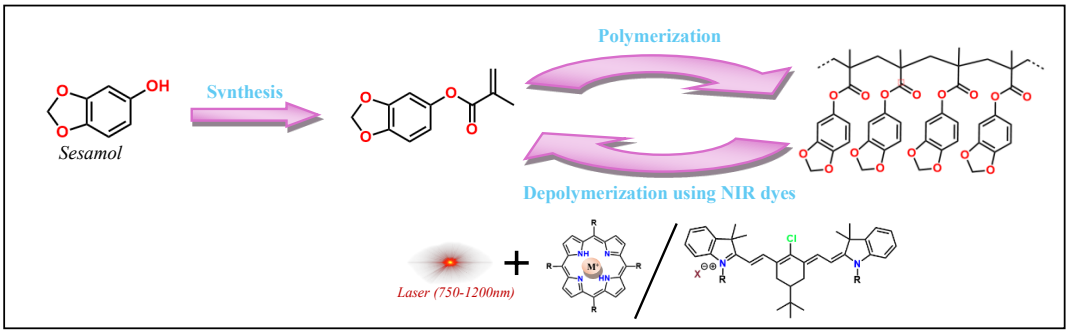

Figure 1 : Polymerization of a biosourced monomer and its depolymerization using an NIR dye

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Cu-Porphyrin Metal–Organic Framework Titania Film Heterojunction for Photocatalysis Applications

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In this era's sustainability goals, solar-light driven water splitting, CO_2 reduction and environmental pollutant remediation have major relevance. Metal–organic frameworks (MOF) with porous crystalline structure have immense potential in photocatalysis due to ultrahigh surface area, numerous active sites and tunable optoelectronic properties. However, their poor e^-/h^+ separation and low charge mobility restrict standalone applications. Construction of step-scheme (S-scheme) heterojunction, featuring an *internal electric field (IEF)* at their interface have shown to improve e^-/h^+ separation and photocatalytic efficiency[1]. Cu-porphyrin MOF with a highly negative conduction band (CB) edge is suitable as reduction photocatalyst (RP)[2] and TiO_2 with a highly positive valence band (VB) edge is suitable for oxidation reaction[3], making them excellent S-scheme partners. A high degree of interfacial contact at OP/RP heterojunction is critical to improve photocatalysis. A high-quality Cu-porphyrin-MOF/TiO_2 heterojunction film with high degree of interface is unprecedented.

Herein, we present microwave-assisted (MWA) solvothermal synthesis of Cu-porphyrin-MOF and its direct-growth on titania film (Cu-MOF/TiO_2 film) with different morphologies (Fig. 1a, e). Firstly we demonstrate uniform 2D- and 1D- Cu-MOF particle morphologies as a function of reaction conditions, such as precursors/modulator mole ratio (Fig. 1b, c). Further, MWA *in-situ* MOF growth on titania film shows well-dispersed cubic-flower morphology with 2D-nanosheet petals (Fig. 1f). Furthermore, MOF growth under atmospheric thermal conditions reveals dendrimer morphology with 1D-rods (Fig. 1g). The significant differences in morphologies could be attributed to structural change of Cu-node secondary-building unit, evaluated through systematic synthesis and physio-chemical characterizations. We observe improved light absorption in Cu-MOF/TiO_2 films ranging from UV to visible light (Fig. 1d). Photocatalysis and photoelectrochemical studies are in progress to evaluate their performance.

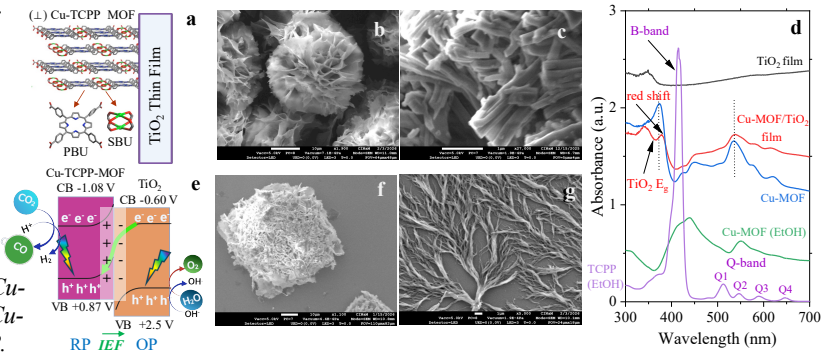

Figure 1: a) Cu-MOF@TiO_2 film; its e) S-scheme heterojunction. SEM of MWA solvothermal grown b) 2D-nanosheet-MOF, c) 1D-rod-MOF and f) Cubic-MOF/TiO_2 film. g) Atmospheric-grown dendrimer MOF/Si. d) UV-Visible spectra of Cu-MOF/TiO_2, pristine Cu-MOF, TiO_2 film and TCPP.

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Hydrochar Modified CuFe Layered Double Hydroxides as Bifunctional Catalysts for Alkaline HER and HOR

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The transition toward carbon-neutral energy systems requires efficient, affordable electrocatalysts to drive both the hydrogen evolution (HER) and oxidation (HOR) reactions. Copper-iron layered double hydroxides (CuFe-LDHs) are promising due to their abundance, tunable redox properties, and Cu-Fe synergy, but their activity remains limited by poor conductivity and surface accessibility[1].

To address these challenges, we developed CuFe-LDH electrodes with functional additives and/or hydrochar (HC). HC, a porous, sp^2-rich carbon derived from pine needles, was introduced to systematically assess its effect on electrode performance, while additional additives were used to tune structural order and ionic mobility.

Electrochemical tests in 1M KOH revealed composition-dependent activity. The best HER and HOR performances were achieved when highly crystalline CuFe-LDH was combined with a hydroxide-conducting ionomer binder. Nevertheless, HC-based electrodes displayed good durability and efficiency in HER and the lowest onset potential during HOR.

These findings confirm that compositional tuning and sustainable hydrochar integration improve CuFe-LDH electrodes for hydrogen technologies, though further optimization is needed to overcome kinetic and mass-transport limitations.

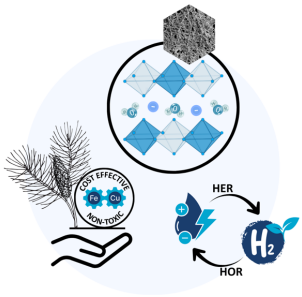

Figure 1. CuFe LDH Nanocomposites for Hydrogen Electrocatalysis

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Bottom-up and top-down strategies for emissive silicates nanocrystals

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Alkaline earth copper silicates with the general formula $ACuSi_4O_{10}$ (where A = Ca^{2+} and Ba^{2+}) represent a family of materials known since antiquity.[1] In particular, $CaCuSi_4O_{10}$ and $BaCuSi_4O_{10}$ traced back in 2500 BC and 1200 BC, and known as Egyptian blue and Han blue, respectively, are characterized by an intense blue color and high stability over time.[2] Besides historical interest, the peculiar layered crystalline structure and their emission in the near infrared region (NIR), makes them interesting new materials for optoelectronic applications.[3] The chromophore group is characterized by a $[CuO_4]$ in a square planar geometry surrounding by $[SiO_4]$ tetrahedra.[4] Recent studies have demonstrated the possibility of obtaining them in nanometric dimensions through exfoliation.[5]
In this work, we present our recent findings on the preparation of colloidally stable 2D nanosheets based on the aforementioned copper silicate compounds. The synthesized nanoplates exhibit an average lateral diagonal of 34 nm and a thickness of 6 nm (Figure 1). Their photoluminescence properties are consistent with those of the bulk material, featuring an excitation maximum at 618 nm and an emission peak at 950 nm. Furthermore, absorbance measurements in cuvettes demonstrate a nearly complete absence of scattering from the suspensions, confirming the high quality and stability of the resulting colloidal dispersions.
This innovative synthetic protocol paves the way for a new class of 2D nanomaterials with promising applications in the fields of biomedical imaging, photovoltaic energy conversion, and IR light-emitting devices. Furthermore, their unique optical properties and stability make them excellent candidates for integration into advanced telecommunication systems.

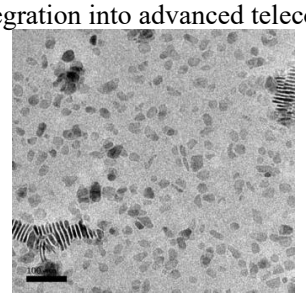

Figure 1 : TEM images of $BaCuSi_4O_{10}$ nanoplates

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Heteroatom-doped carbon quantum dots as selective electrocatalyst for the reduction of CO_2

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Electrochemical CO_2 reduction (ECO_2R) offers a promising route for mitigating climate change by converting CO_2 into valuable chemicals and fuels. Realizing this potential requires the development of efficient, stable, and low-cost catalysts. In this work, we synthesize heteroatom-doped carbon quantum dots (CQD) via a hydrothermal process using abundant, non-toxic precursors such as citric acid, glucosamine and cysteine. Combined with a long-chain anion-exchange ionomer, these CQD-based materials were evaluated as electrodes for ECO_2R.

CQD derived from citric acid exhibit excessive hydrophilicity, leading to dominant hydrogen evolution. In contrast, Cu,S,N-CQD synthesized from glucosamine show markedly improved activity and selectivity. Their performance arises from a synergistic combination of features: a high electrochemically active surface area that provides abundant CO_2 activation sites; an optimal nitrogen content, particularly in aminic and pyridinium-oxide positions, that enhances CO_2 adsorption; an appropriate amount of Cu species that promotes C–C coupling and acetate formation; and sulfur in multiple oxidation states that further boosts catalytic activity.

The resulting electrodes achieve a mass-specific acetate production rate of 1.5 mmol g^{-1} h^{-1}, surpassing previously reported CQD-based catalysts. Faradaic efficiencies exceed 45% across a wide potential window (0 to −0.4 V vs RHE) and reach 68% at −0.2 V. Owing to the low overpotential, the energy efficiency is high: 52% for acetate at −0.2 V, ranking among the best values reported.

Overall, these results demonstrate that Cu,S,N-doped CQD derived from glucosamine constitute a highly promising class of ECO_2R electrocatalysts. Their combination of low-cost, environmentally benign precursors, high acetate selectivity, and excellent energy efficiency highlights their potential for advancing practical CO_2 electroreduction technologies.

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Copper-Modified Hydroxyapatite Surfaces as Catalysts in Environmental Processes: A Computational Perspective

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In recent years, hydroxyapatite (HA, $Ca_{10}(PO_4)_6(OH)_2$) has emerged as a promising material in green chemistry, owing to its feasible synthesis from waste-derived resources. [1] Its tunable acid-base properties, non-toxicity, adsorption capability, and ion-exchange behaviour, make HA an attractive support for eco-friendly heterogeneous catalysts aimed at the abatement of environmental pollutants. [2] In this context, the nature and strength of molecule-surface interactions play a key role in determining catalytic performance. Computational methods have therefore become an essential tool to accurately describe these interactions and to support rational catalyst design, [3] benefiting from the continuous advancement in computational power. [4]

In this contribution, a periodic quantum mechanical approach is employed to investigate the interaction between small reactive molecules and the most stable hydroxyapatite surfaces. Copper-modified HA models are considered to enhance catalytic activity while preserving the structural integrity of the material. [5] Specifically, the interaction of formaldehyde, taken as a benchmark volatile organic compound, with the (001), (010), and (101) HA facets is analysed for both pristine and Cu-substituted surfaces. In addition, ammonia selective catalytic reduction (NH_3-SCR) is examined in comparison with experimentally driven data, with particular attention to the effect of water. Variations in structural, energetic, and vibrational properties are discussed to establish a computational framework for the investigation of environmentally relevant catalytic processes. This approach can be readily extended to other cationic substitutions, such as iron, highlighting hydroxyapatite as a versatile and highly promising material for environmental catalysis.

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OH-initiated Oxidation and Photochemical Degradation of Muconaldehyde: a Computational Study using DFT and Coupled Cluster Methods

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2,4-hexadienaldehyde (muconaldehyde) is an unsaturated dicarbonyl compound of significant environmental and toxicological interest, derived mainly from the oxidation of benzene.[1] Despite its environmental and toxicological relevance — being associated with the formation of photochemical smog, secondary organic aerosols and severe myelotoxic effects — its chemical kinetics in the atmosphere have not yet been fully characterized.[2] This theoretical study aims to clarify the degradation pathways of the molecule initiated by the OH radical and photochemically through DFT (M06-2X/def2-TZVP), with energy refinements at the DLPNO-CCSD(T)/def2-TZVP level. TD-DFT (O3LYP/def2-SVP) methods were used to study the excited processes and intersystem crossing constants.
The study of the reaction with the OH radical revealed close competition between the aldehyde hydrogen extraction pathway and the double bond addition pathway (Figure 1), with extremely close energy barriers, while for photochemical processes, this study highlighted the importance of intersystem crossing processes, revealing that this shift occurs extremely rapidly on the T_1 triplet surface, with a kinetic constant of $9{,}7 \cdot 10^9$ s^{-1}.
These results lay the foundations for future studies aimed at outlining a global picture of the degradation of this molecule under real atmospheric conditions.

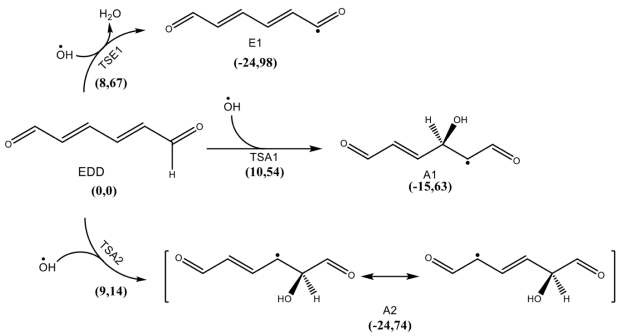

Figure 1: Reactivity of E,E-2,4-hexadienedial with the OH radical: initial reaction steps. Free energies are calculated at level CCSD(T)/def2-TZVP//M06-2X/def2-TZVP, expressed in kcal mol^{-1} at 298 K.

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P-41

De novo acyl carrier proteins display structure-independent modification and sequence novelty

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Acyl carrier proteins (ACPs) are dynamic, structurally conserved α-helical proteins central to many primary and secondary metabolic processes. Whilst prior engineering efforts have focused on strategic mutagenesis and "helix swaps", much of the ACP sequence design space remains underexplored. In this study, diverse variants of the archetypal ACP subclass – AcpP – were created, using a bespoke sequence-generating algorithm (ALGO-CP). Among these, two soluble candidates – ALGO-055 and ALGO-059 – were generated and shown to undergo full post-translational modification from *apo*→*holo*→acyl forms *in vitro*, using recombinant modifying enzymes. To investigate the structural behaviour of these designed sequences, molecular dynamics simulations were performed on their three forms (*apo*, *holo*, and *acyl*) in order to examine how their secondary structure evolves over time. The results were compared with simulations of two reference ACP crystal structures from *Escherichia coli* and *Helicobacter pylori*. The *in silico* results indicate that the *holo* ACPs are intrinsically less stable than their corresponding *apo* counterparts, with the notable exception of the ALGO-055 variant, which remains structurally stable in both *apo* and *holo* states. Experimental observations, however, suggest that some key aspects of ACP behaviour – specifically, post-translational modification – can be retained independently of the canonical structure. Overall, this work establishes a foundation for probing ACP sequence diversity through a hybrid computational-experimental approach.

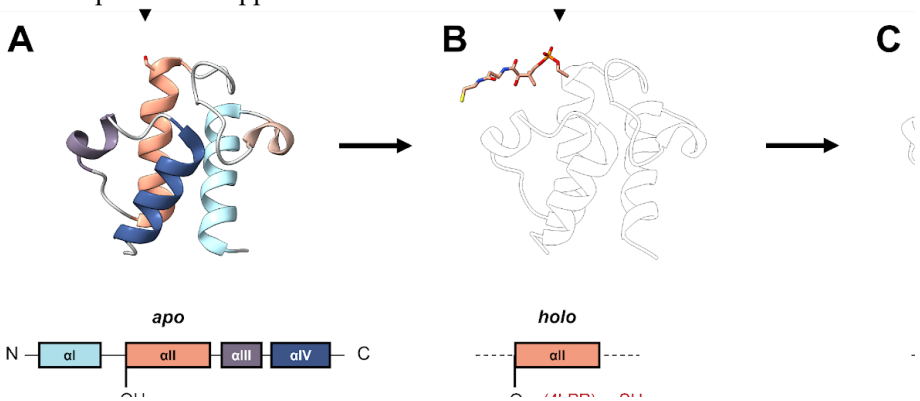

Figure 1: (A-C) Annotated schematic of an ACP, with colour-coded α-helices, in its apo (A), holo (B) and acyl (C) state. (PDB: 1T8K, 5H9H and 2FAE). Black triangles indicate the position of the invariant, essential serine.

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Opuntia ficus-indica L. cladodes gel as a solvent medium for natural formulations

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In the context of natural products extraction, the use of edible solvents offers an alternative approach to conventional organic solvents. In addition to providing a non-toxic, natural option, this method eliminates the need for solvent evaporation, allowing direct incorporation of the extract into bio-based formulations. The aim of this study was to evaluate the feasibility of using cactus gel (*Opuntia ficus-indica* mucilage) as an edible solvent for extracting valuable compounds. Accordingly, two approaches were investigated: (a) the solubilisation of compounds with application potential and their formulation into a test product, and (b) in-plant extraction from Opuntia flowers and evaluation of suitable preservation methods.
The gel was recovered on a lab scale, and its composition, as well as its chemical and physical properties, were studied in both raw and preserved states.
In the first part of this study, solubilisation experiments were carried out on caffeine, menthol and aescin. All these substances have potential applications in cosmetics. Curves were produced to study the percentage solubilised as a function of temperature and were compared to water as a reference solvent. Subsequently, a body gel was formulated.
In the second part, the solvent capacities during extraction were examined using the flowers of *Opuntia ficus-indica*, with the aim of performing an in-plant extraction, where both the solvent and the matrix originated from the same plant. Extraction using the gel as a solvent was performed using three different techniques: dynamic maceration, infusion under agitation at 50 °C, and ultrasound-assisted extraction. All extractions were conducted using a solid-to-liquid ratio of 1:30, with extraction times set at 15 and 30 min. For comparison, similar extractions were carried out using water and a mixture of ethanol and water (70/30 v/v) as solvents. Following the extractions, preservation methods were tested and compared by monitoring, over two weeks, the gel, the preserved gel, the ultrasound extract and its preserved version, and their evolution.
The phenolic fraction of the extracts and the gel was analysed by liquid chromatography-mass spectrometry (LC-MS). The total phenolic content was found to be similar in both extracts obtained by gel and hydroalcoholic extraction. In-depth analysis of the chromatograms further confirmed the potential use of the gel as a viable and edible solvent for the extraction of valuable compounds.

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From polyamines to nanogels: a supramolecular approach for boosting relaxivity of $[Gd(DOTP)]^{5-}$

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Supramolecular chemistry has played a central role in advancing the development of more effective contrast agents (CAs) for magnetic resonance imaging (MRI).[1] By incorporating Gd(III) complexes into larger supramolecular architectures, host–guest interactions can be exploited to enhance both performance and targeting. Optimizing these interactions has the potential to substantially increase longitudinal relaxivity (r_1), thereby improving MRI signal enhancement and enabling lower administered doses without compromising image quality.
In this work, we investigated the formation of ion pairs between the anionic complex $[Gd(DOTP)]^{5-}$, which lacks an inner-sphere water molecule, and cationic polyamine substrates such as cyclen, octaazacryptand, and low-molecular-weight polyethyleneimine (PEI). Our approach combines ^{1}H NMR relaxometric techniques with DFT calculations.[2] Relaxometric titrations of dilute $[Gd(DOTP)]^{5-}$ solutions with increasing amounts of the cationic substrates allow determination of the ion-pair binding constants as well as the relaxivity of the resulting supramolecular adducts. The strength of these interactions increases with the number of positive charges on the polyamine and depends strongly on pH, reflecting the optimal balance of charges between anion and cation. With cyclen, at pH 9.0, $[Gd(DOTP)]^{5-}$ forms a 1:2 adduct (one Gd-complex to two cyclen units), increasing relaxivity to 9.0 $mM^{-1}s^{-1}$ (32 MHz and 298 K). The most significant boost among the polyamines was observed with PEI at pH 7.2. The flexible polymer chain allows for a very strong interaction (K = 1.8 x 10^4 M^{-1}) and multiple binding sites (n ≈ 6.4), leading to a relaxivity of 27.0 $mM^{-1}s^{-1}$ at 32 MHz and 298 K. A further and remarkable enhancement in relaxivity is observed when the metal complex is confined within nanogels. Analysis of the corresponding NMRD (Nuclear Magnetic Relaxation Dispersion) profiles highlights the essential contribution of well organized second-sphere water molecules with restricted mobility, which are responsible for the unusually high relaxivity values at magnetic fields relevant for MRI.

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Design and Synthesis of Pyrazolo[3,4-*d*]pyrimidine Derivatives as Potential Src Kinase Inhibitors

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Src is a non-receptor tyrosine kinase and the first identified proto-oncogene, playing a crucial role in tumor progression, metastasis, and therapy resistance. Its overexpression has been reported in several malignancies, including triple-negative breast cancer, glioblastoma, and pancreatic cancer, making Src an attractive target for anticancer drug development.
Pyrazolo[3,4-*d*]pyrimidines are nitrogen-containing heterocycles widely investigated as kinase inhibitors. Early compounds such as PP1 and PP2 are commonly used as reference inhibitors in kinase studies. More recently, SI306(1) and SI113(2) have been identified as potent inhibitors of Src and SGK1, respectively. Starting from these scaffolds, new derivatives were designed to explore structure–activity relationships (SAR) and identify novel Src-targeting agents.
In this work, a series of pyrazolo[3,4-*d*]pyrimidine derivatives was synthesized through a multistep synthetic approach. Key intermediates were obtained from styrene oxide derivatives reacted with hydrazine monohydrate, followed by condensation with ethyl(ethoxymethylene)cyanoacetate and cyclization to afford the pyrazolo[3,4-*d*]pyrimidinone core.
Subsequent functionalization at positions 4 and 6 generated a small library of analogues bearing different substituents. In particular, allyl groups were introduced at position 6 to enable potential conjugation with halloysite(3), a strategy aimed at improving in vivo drug delivery. The synthesized compounds are currently under evaluation for enzymatic inhibition and antiproliferative activity.

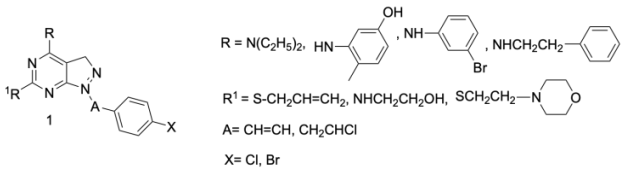

Figure 1. General structure of the synthesized pyrazolo[3,4-d]pyrimidine derivatives.

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Glutaminase 1 (GLS1) allosteric inhibitors: synthesis of key intermediates

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In recent years, glutamine metabolism has emerged as a promising hallmark in cancer research, as many tumor cells rely on this amino acid to sustain their growth and survival. Glutamine serves as a major energy source after glucose for cancer cells, playing an important role in supplying the tricarboxylic acid (TCA) cycle and supporting the biosynthesis of lipids, amino acids, and nucleotides. Consequently, the inhibition of glutamine metabolism arrests tumor growth and induces cancer cell death [1].

Glutaminase (GLS), the rate-limiting enzyme of glutaminolysis, represents an attractive therapeutic target for the development of antiproliferative agents. GLS exists as GLS1 and GLS2 isoforms with distinct splice variants and tissue distributions. Resulting overexpressed in several tumors, GLS1 has become the main focus of research due to its role in cancer development [2].

Two major classes of GLS1 inhibitors, based on their different biding sites, have been developed: active-site and allosteric inhibitors [3]. The first class, represented by DON, showed strong antitumor activity but its clinical use was limited by its off-target toxicity [4]. The reversible allosteric inhibitors, such as BPTES, exhibited improved specificity and safety by binding to GLS1 activation loop. Despite promising preclinical activity, BPTES exhibits poor aqueous solubility and metabolic stability, and low bioavailability [5]. Indeed, only two BPTES-derived compounds (**CB-839** and **IPN60090**) have advanced to clinical trials, [6, 7], highlighting the need for further optimization of GLS1 inhibitors for effective cancer therapy.

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Determination of water content in vanilla pods and powder using near-infrared spectroscopy

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The quality of vanilla depends heavily on its water content, a key parameter that influences its stability, preservation, and sensory properties. Conventional moisture determination by loss-on-drying, while accurate, is slow and destructive. In this study, a rapid, non-destructive approach based on near-infrared (NIR) spectroscopy combined with chemometric modeling was developed to predict the moisture content of vanilla samples. A total of 123 samples were analyzed by NIR spectroscopy and thermogravimetric analysis (reference values). Principal component analysis revealed a strong correlation between spectral variance and water content in the 7400-4000 cm^{-1} region. A partial least squares (PLS) regression model was optimized and validated, showing optimal performance with four latent variables (R^2 = 0.99, RMSEC = 0.98). Prediction on an independent set of 20 samples yielded a Q^2 of 0.99 and an RMSEP of 0.82, confirming the robustness and generalization of the model. Repeatability tests further demonstrated high stability and low variability of the predicted values. The method demonstrates strong potential for routine industrial quality control. Expanding the calibration set could support broader applicability across vanilla varieties.

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P-47

Design, synthesis and biological evaluation of RNA ligands targeting the SAM I/IV riboswitch

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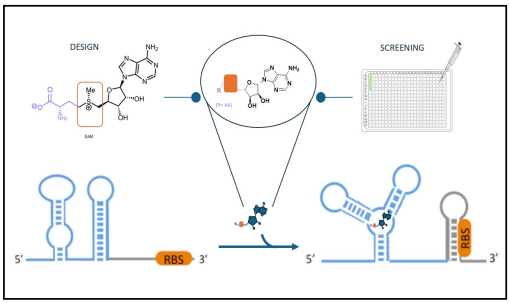
The global rise of antibiotic resistance underscores the urgence of new validated cellular targets to advance antibacterial drug discovery[1], and targeting RNA now rises as a promising approach in medicinal chemistry. Riboswitches (RBS) align well with the growing shift from traditional protein targets toward structured regulatory RNAs, as they directly control essential bacterial genes through selective metabolite binding[2]. Among these, SAM-binding riboswitches regulate conserved pathways critical for bacterial viability, making the SAM riboswitch a promising target.[3]

In this context, the project aims to develop small molecules with potential antibacterial properties, beginning with the rational design of SAM analogues. The synthetic approach, starting from adenosine acetonide, initially focuses on linker modification and follows an established 3–6 step flexible strategy that allows the synthesis of a broad series of derivatives while keeping the same core reactions, thereby facilitating the exploration of chemical diversity around the target scaffold.

The resulting compounds are screened via fluorescence-based assays, enabling the assessment of affinity/selectivity and, thus, the identification of potential hits. The most promising candidates are subjected to structure-activity relationship optimization and consequently evaluated via microbiological assays, including *in vivo* studies, with the goal of achieving new bioactive molecules and ultimately contributing to the development of next-generation antibacterial agents.



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Design and Synthesis of Cysteine-Targeting Covalent Inhibitors Bearing an α,β-Unsaturated Ketone Warhead

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The study of Targeted Covalent Inhibitors (TCIs) has provided a transformative approach in drug discovery, offering prolonged target engagement and the ability to overcome drug resistance issues. Among nucleophilic amino acids, cysteine residue remains the gold standard for covalent modifications due to its unique reactivity and strategic conservation in numerous therapeutic targets[1]. A critical challenge in TCI design is correctly design the molecular structure allowing the engagement of selective *non*-covalent interactions within the target binding pocket, ensuring high affinity and proper orientation of the warhead toward the target cysteine residue[1].
In this work, we propose the design of an enzymatic inhibitor featuring an α,β-unsaturated ketone as Michael acceptor warhead that offers reactivity towards a cysteine residue present in the active site of our target enzyme[2]. The design started from a previously disclosed inhibitor, known for its affinity toward the target of our interest, that was modified by introducing the electrophilic warhead.
In this work, the synthesis of a compound as possible TCI is proposed and discussed. This synthetic route provides a flexible tool to build a library of compounds containing the proposed moiety in order to identify compounds with enhanced affinity for the target enzyme.

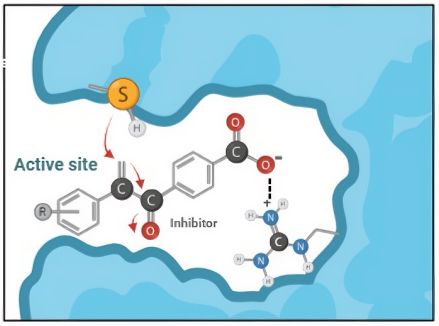

Figure 1: Interaction of the proposed electrophilic moiety with the target cysteine

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P-49

Adressing oncoproteins to the lysosome using synthetic chimeric molecules

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Inhibition of oncogenic proteins has long been a cornerstone in the treatment of leukemia. However, the emergence of treatment resistance due to mutations in these targets has spurred the development and rapid advancement of targeted protein degraders, such as PROTAC technology. Our objective is to develop an innovative approach using ADOLYS compounds to directly address oncogenes to lysosomal degradation through the Chaperone Mediated Autophagy (CMA) process. These ADOLYS compounds are precisely designed chimeric molecules that intricately connect two proteins, the chaperone protein HSC70 necessary for lysosomal delivery and the oncogenic target protein.
Acute Myeloid Leukemia (AML) frequently involves mutations in the FMS-like tyrosine kinase 3 (FLT3) gene, found in about 30% of AML cases. The most prevalent mutation is the internal tandem duplication (FLT3-ITD), present in approximately 25% of AML cases. This mutation drives the disease, leading to a high leukemic burden and poor prognosis. Effective treatment has been characterized by inhibiting the BTK protein kinase, which acts downstream of FLT3-ITD, using Ibrutinib. Our approach aims to degrade BTK, a critical oncogenic target in this condition.
To achieve this, we propose synthesizing a chimeric compound that merges an anchoring motif for the chaperone protein HSC70 with a BTK protein inhibitor. The goal is to use the chaperone-mediated autophagy (CMA) process to specifically degrade the BTK protein kinase. The development of this heterobivalent construct involved multiple optimization cycles across several generations of ADOLYS degraders. Key steps included HSC70 recognition motif screening, in cellulo evaluation of efficacy, and extensive scaffold optimization encompassing heterobivalent molecule design, physicochemical tuning, and structural modifications to enhance cellular delivery.

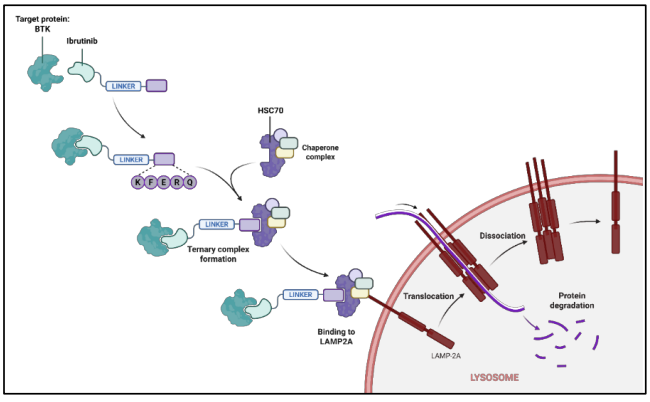

Figure 1: Addressing BTK to the lysosome using ADOLYS heterobivalent compound

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P-50

New biological investigations on triazol-imidazo[1,2-*b*]pyrazole scaffold

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The 1,2,4-triazole scaffold is a key pharmacophore widely present in a broad range of biologically active compounds, including anticancer agents [1]. In previous studies, we demonstrated the potential of the 1,2,4-triazole nucleus when linked to an imidazo-pyrazole scaffold for the design of biologically active compounds [2,3]. In particular, compounds **1** (Figure 1) showed significant anticancer activity, especially against melanoma cell lines, thus confirming the medchem attractiveness of the triazol-imidazo[1,2-*b*]pyrazole core [4].

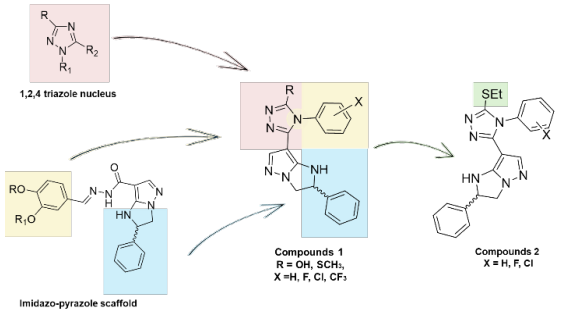

*Figure 1: Structure of previous derivatives **1** and new functionalized compounds **2***

To further extend the structure-activity relationships (SARs) of **1**, we designed and synthesized novel analogues **2** (Figure 1) in which the triazole nucleus was functionalized with a more embedded thioethyl substituent. The new compounds were evaluated for anticancer activity across different cancer cell lines and for the inhibitory effects on aggregation and ROS production on human platelets that represent a good biological model to assay potential anti-inflammatory and anticancer drugs. The synthetic approach, the biological data and the derived SARs will be discussed in the poster.

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Design and synthesis of new prolyl isomerase Pin1 inhibitors against aggressive tumors

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Peptidyl-prolyl *cis-trans* isomerase Pin1 is a key regulatory enzyme that catalyzes the *cis–trans* isomerization of phosphorylated Ser/Thr-Pro motifs in proteins, modulating several cellular signalling pathways. Pin1 overexpression is strongly associated with tumour initiation, progression, metastasis and therapy resistance, making it an attractive target for anticancer drug development. [1]

Among known Pin1 inhibitors, *all-trans retinoic acid* (ATRA) binds the catalytic PPIase domain, inhibiting enzymatic activity and promoting Pin1 degradation. However, several limitations restrict its broader therapeutic use, highlighting the need for new analogues with improved properties. [2] Structural studies indicate that the carboxylic acid group of ATRA forms key ionic interactions with Lys63 and Arg69 residues in the Pin1 active site. [2] Based on this information, bioisosteric replacement approach has been applied to identify promising acidic scaffolds capable of establishing key interactions within the Pin1 active site while modulating the physicochemical properties of the molecules. [3]

Computational studies, including molecular docking and molecular dynamics simulations, have been used to validate the compound design. Target molecules were synthesized through suitable synthetic routes and evaluated *in vitro* for their ability to inhibit Pin1 enzymatic activity. In this context, the design, synthesis and biological evaluation of a series of target compounds will be described and discussed.

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