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Welcome to the 22nd edition of the Merck Young Chemists' Symposium (MYCS), formerly also known as SAYCS and MEYCS. This international conference is organized by the Young Group of Società Chimica Italiana (SCI Giovani) and the National Interuniversity Consortium of Materials Science and Technology (INSTM) with the financial support from Merck and several other sponsors, that you will meet during the conference.

The symposium covers all the disciplines of Chemistry, aiming to connect young researchers, inspire new ideas, and potentially trigger new collaborations. With the contributions of our five invited plenary speakers, and the international environment guaranteed by the presence of people coming from different countries, we truly hope that you will all enjoy this great event with us. We have worked hard to organize this meeting with 230 participants, prioritizing high-level scientific topics and other themes of crucial importance in our modern society. Thank you for the great trust shown towards SCI Giovani, Merck and all our supporters. Enjoy the conference and have a nice stay with us!

Marta Da Pian

Marta Da Pian
SCI Giovani Coordinator

MYCS 2023

RIMINI | 13-15 NOVEMBER 2023

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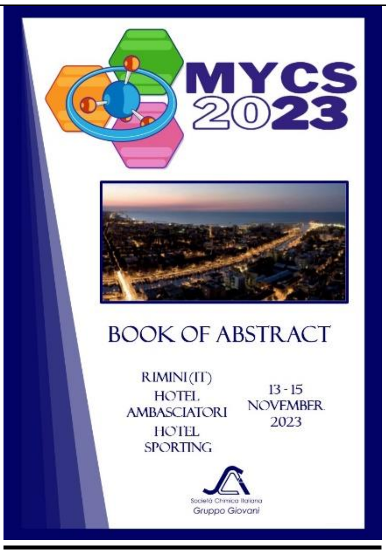 MYCS 2023 BOOK OF ABSTRACT RIMINI (IT) HOTEL AMBASCIATORI HOTEL SPORTING 13 - 15 NOVEMBER 2023 Società Chimica Italiana Gruppo Giovani	All the scientific contributions of the symposium are collected in this international volume with ISBN code. You can cite your work as follows: N. Surname, N. Surname, g and N. Surname, <Abstract title>, in Proceedings of the Merck Young Chemist’s Symposium 2023, XXII Ed. I. Arduino, C. Bonfio, M. Bonomo, M. Da Pian, A. Dall'Anese, A. M. Fiore, E.F. Gulino, A. Malara, M. Mendolicchio, C. M. Montone, E. Paone, A. Polo, L. Rivoira, A. Rossetti, I. Romeo, M. Salzano de Luna, S. Tortorella, F. Vincenti. ISBN: 978-88-94952-44-5, <page number>, 2023, Rome.

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PL01

Making the Leap: A Journey from Academia to Industry

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An overview of the exciting and challenging journey from academia to industry will be presented, highlighting key themes and insights for those considering or embarking on the transition from academia to industry, which is a transformative and often daunting endeavor. This presentation explores the pivotal factors and personal experiences involved in making this leap.

As academic researchers increasingly seek opportunities beyond traditional academic paths, the shift to industry is a compelling option, presenting new challenges and exciting prospects. The transition begins with recognizing the need for change and embarking on a journey of self-discovery. Challenges and uncertainties are an inherent part of this journey. Early career academics must adapt to a faster-paced environment, translate their specialized knowledge into practical solutions, embrace multidisciplinary collaboration, cultivating business acumen, and developing an entrepreneurial spirit.

The importance of cultivating soft skills, including communication, project management, and adaptability, to excel in this evolving landscape will be underscored.

The allure of industry lies in its potential for real-world impact and financial reward, but this path requires a shift in mindset, as well as a commitment to continuous learning and development. Navigating the world of patents, regulatory compliance, and customer demands can be complex, but it offers unique opportunities for personal and professional growth. The importance of preparation, networking, and mentorship as crucial tools for success will be emphasized.

Early career scientists will be encouraged to cultivate a proactive approach to their career development, embracing the journey from academia to industry as an opportunity for personal and professional growth.

PL02

SeedScience - science education from the African continent

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Teaching science in a practical, simple and fun way can be complicated. There are contexts in which this is particularly true. The non-profit association SeedScience works in some African countries to change this trend. It trains science teachers and collaborates with them to provide quality education for their students. It develops engaging and sustainable educational activities, collaborates with schools and communities, and uses creativity to inspire curiosity, stimulate critical thinking, and promote scientific awareness among young people.

In the past 5 years, SeedScience trained more than 150 science teachers across African countries improving the quality of education for more than 12.000 students from grade 10 to 12.

Figure 1: Students in Tanzania during a science experiment. Photo by Roberta Baria.

PL03

Colloid Chemistry: A Way to Design Functional Hybrid Nanomaterials

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Colloid Chemistry has always been an integral part of several chemical disciplines. Ranging from preparative inorganic chemistry to physical chemistry, a great scientific interest was aroused by the dimensions and the possibilities colloids offer. With the advent of nanotechnology and analytical tools, which evolved across recent decades, colloid chemistry has become essential for high-level research in various fields.

In particular, it deals with the synthesis of various colloidal structures in the nanometer range, including inorganic and metallic nanoparticles, macromolecular structural units, amphiphiles and their supramolecular organizations, as well as emulsions and foams.

Colloid Chemistry can represent an intriguing way to design and create a huge set of new multifunctional nanomaterials with a structural hierarchy and with a large spectrum of known and as yet unknown properties. These ones can fulfil very specialized tasks for several (bio)technological applications, from photocatalysis to energy generation, from biomedicine and food chemistry to sensing and optoelectronics. Here, organo-inorganic hybrid nanomaterials can be designed and realized through bottom-up wet-chemistry routes, starting by the molecular precursors of both inorganic and organic phases thus leading to hybrid nano-systems exerting peculiar functionalities.

In this talk, an overview of multifunctional hybrid nanomaterials for biomedical and environmental applications is proposed. Following a bioinspired approach, they have been obtained by combining inorganic colloidal nanocrystals, such as metals or metal oxides, alternatively with bioderived macromolecules, such melanins [1,2] and polyphenols [3,4], and amphiphilic molecules, such as lipids and long-chains fatty acids [5,6]. A combined approach of spectroscopic and scattering techniques lead to define the main physicochemical features of such multifunctional nanomaterials.

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[3] G. Vitiello et al., *Environmental Research* 193 (2021) 110562
[4] V. Venezia, G. Vitiello et al., *Journal of Environmental Chemical Engineering* 11 (2023) 108973
[5] A. Luchini, G. Vitiello et al., *Frontiers in Chemistry* 7 (2019) 343
[6] N. Gallucci, G. Vitiello et al. *Nanomaterials* 11 (2021) 542

PL04

Precision medicine journey through omics approach

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The rise of technologies simultaneously measuring thousands of data points represents the heart of systems biology. These technologies have significantly impacted the discovery of next-generation diagnostics, biomarkers, and drugs in the precision medicine era. Driven by high-throughput omics technologies and the computational surge, it enables multi-scale and insightful overviews of cells, organisms, and populations. Precision medicine capitalizes on these conceptual and technological advancements and stands on two main pillars: data generation and data modeling. High-throughput omics technologies allow the retrieval of comprehensive and holistic biological information, whereas computational capabilities enable high-dimensional data modeling and accessible and user-friendly visualization.

Furthermore, bioinformatics has enabled comprehensive multi-omics and clinical data integration for insightful interpretation. Despite their promise, translating these technologies into clinically actionable tools has been slow [1].

In this plenary talk, I will give an overview of the main trends in this field, with a particular focus on what is studied in my research group at Sapienza University of Rome and on how it impacted my career since 2012. The potential and meaning of omics data, including proteomics, peptidomics, and metabolomics, will be discussed with some peculiar examples. In particular, the concept of the protein corona will be discussed to create new opportunities for diagnostic and personalized nanomedicine [2], as well as multi-omics digital platforms for advancing precision medicine for prostate cancer for the identification of key diagnostic and prognostic biomarkers in tissues and biological fluids of patients with prostatic carcinoma [3].

[1] C.B. Clish, *Mol Case Stud* 1 (2015) a000588.
[2] L. Digiacomo, K. Jafari-Khouzani, S. Palchetti, Capriotti et al, *Nanoscale* 12 (2020) 16697–16704.
[3] A. Cerrato, C. Bedia, A.L. Capriotti, et al., *Anal Chim Acta* 1158 (2021) 338381.

PL05

Electrochemistry meets light: Electrochemiluminescence-based biosensors from academic curiosity to an industrial success

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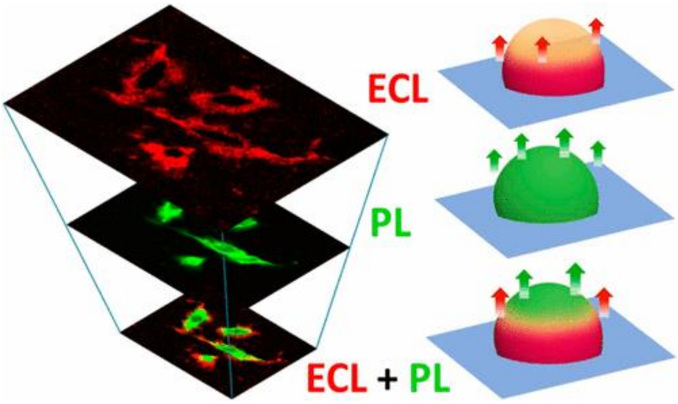
If you want to admire the Milky Way in all its splendor, you should choose a moonless (and possibly romantic) night, away from urban light pollution. Analogously, if you need to quantify an analyte in a very low concentration you need to work close to zero background. Electrochemiluminescence (ECL) is a marriage between photochemistry and electrochemistry and is a leading technique in bioanalysis [1]. Since the excited species are produced with an electrochemical stimulus rather than with a light excitation source, ECL displays an improved signal-to-noise ratio compared to photoluminescence [2]. The electrochemically-induced way to generate luminescence signal allows to obtain sensors with low background, high sensitivity, good temporal and spatial resolution, robustness, versatility, and low cost. As a matter of fact, ECL has become a powerful analytical technique widely studied and applied both from the academic and industrial point of view. If we have a look at the last 20 years, the number of scientific publications focused on ECL research has been exponentially increased and commercial clinical analyzer, Elecsys®, is an industrial success.

In the quest for ever-increasing sensitivities, ECL can ideally be coupled to nanotechnology for developing new systems and strategies for analyte determination. In this context, thanks to the combination of different nanomaterial we were able to “fuel” the generation of the ECL reagents and optimize its interaction with the dye reaching very competitive limits of detection in complexes matrix such as blood and urine [3]. Our last efforts have been focused also in the combination between ECL and microscopy for single cells analysis with high throughput and low detection limit [4] and for the point of care PCR-free Hepatitis B Virus determination.



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[4] a) G. Valenti, et al., *J. Am. Chem. Soc.* 139 (2017) 16830-16837; b) S. Voci, et al. *J. Am. Chem. Soc.* 140 (2018) 14753−14760; c) A. Zanut at al G. Valenti, F. Paolucci, *Nature Commun.* 11 (2020) 2668; d) A. Zanut et al, *Angew. Chem. Int.* Ed. 59 (2020) 21858 –21863

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OR75 – Botto Asia (UniPI)

OR01

Development of a salivary uric acid sensor for health status monitoring

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Domenica Tonelli,[a] Danilo Arcangeli,[a] Isacco Gualandi,[a] Beatrice Fraboni,[b] and Erika Scavetta[a]

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Uric acid (UA) is a relevant biomarker associated with health status. In particular, it is the major antioxidant component in saliva so UA concentration can be exploited to estimate oxidative stress [1]. This disorder is defined as a disturbance in the balance between the production of reactive oxygen species (free radicals) and antioxidant defences and has been linked to a wide range of health problems including cancer, cardiovascular and neurodegenerative diseases. In this contribution, we present the development of a chemical sensor based on organic electrochemical transistor (OECT) transduction mechanism for uric acid selective monitoring in saliva, exploiting potentiodynamic technique to guarantee selectivity, using transconductance peak (gm) as the analytical signal (Fig.1). Sensors are fabricated with poly(3,4-ethylenedioxythiophene):polystyrene sulfonate (PEDOT:PSS) thus benefitting of the polymer capability to catalyze analytes electro-oxidation. UA is detected with the OECT sensor, by means of its oxidation occurring at a gate voltage within PEDOT:PSS stability window [2]. Device structure and performances were optimized resulting in a sensitivity of (62 ± 5) μS dec^{-1}, high repeatability and reproducibility, respectively 5% and 8% expressed as relative standard deviation, and a limit of detection of 1 μM. The measures were then carried out in human and pig saliva, showing the possibility to exploit the device for analysing real, complex and destructive matrices. The results were compared to a commercial enzymatic assay kit for salivary uric acid: UA concentration in human saliva estimated with OECTs was statistically equivalent to the one assessed with the commercial kit ($(3.4 \pm 0.2) \times 10^2$ μM) demonstrating the accuracy of the detection and validating the method. The small, light-weight devices can be easily integrated into portable electronics to further simplify the setup and reduce costs.

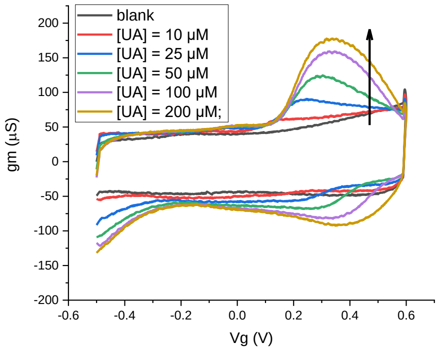

Figure 1: Transconductance curves at increasing uric acid concentration.

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[2] D. Arcangeli et al., *ACS Sensors*, 8 (2023) 1593–1608

OR02

Highly sensitive chemoresistive sensors based on Cu/Pd-doped CeO_2 for hydrogen detection at room temperature

Alberto Cerchiai,[a] Elena Eremeeva,[a] Federico Maria Vivaldi, [a] Andreas Güntner,[b] and Fabio di Francesco[a]

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Hydrogen is considered the most promising energy vector of the future, capable of replacing fossil fuels. Its use is expected to significantly increase in the next decades, but several safety issues have to be dealt with. In fact, hydrogen is a potentially dangerous gas, especially in the event of leaks, due to its high diffusive coefficient and wide explosion limits in air (4 – 75 % v/v) [1]. For these reasons, the development of reliable and accurate sensors for the detection of leaks will play a crucial role in fostering and supporting a larger use of this gas. Hydrogen detection is also widely employed in breath analysis to diagnose bacterial infections or lactose intolerance [2]. In fact, hydrogen is produced in the digestive tract of intolerant individuals through bacterial metabolic processes. In this work, we present a chemoresistive sensor based on pure or Pd/Cu-doped CeO_2 synthesized through Flame Spray Pyrolysis (FSP), a technique that allows the synthesis of nanoparticles through the combustion of organic metal precursors using a methane-fed flame [3]. Pure and Pd/Cu doped cerium oxides were characterized by XRD and BET, and directly deposited via FSP on interdigitated electrodes on Al_2O_3 substrates. The resulting CeO_2 layers were porous and thermally, chemically, and mechanically stable. After the annealing at 500°C for 5 h, the sensors were tested with different gaseous analytes. Sensors with pure CeO_2 were selective for methanol over ethanol and for xylene over toluene and benzene. On the other hand, Pd-doped CeO_2 sensors proved to be sensitive to hydrogen, able to work at room temperature and not affected by any known interferents. Furthermore, thanks to the ability to detect extremely low concentrations of hydrogen in the air, down to 150 ppbV, the Pd-doped CeO_2 sensor is suitable for use both for the preventive detection of hydrogen leaks and for the diagnosis of food intolerance via breath analysis.

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[2] C. De Geyter, K. Van de Maele, B. Hauser, and Y. Vandenplas, *MDPI* (2021) 1-8
[3] L. Mädler, H. K. Kammler, R. Mueller and S. E. Pratsinis, *J. Aerosol Sci.* 33 (2002) 369–389

OR03

Photoelectrochemical detection of ciprofloxacin using a mesoporous silica/AuNPs/TiO_2 hybrid electrode

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In recent years, the development of electrochemical sensors has gained significant attention due to their potential applications in various fields, including environmental monitoring, biomedical diagnostics, and food safety. The increasing occurrence of antibiotic residues in environmental samples and their potential adverse effects on human health and ecosystems necessitate the development of sensitive and selective detection methods. The proposed electrochemical sensor offers a promising solution by leveraging the unique properties of mesoporous silica, gold nanoparticles (AuNPs), and TiO_2 to enhance the detection of ciprofloxacin.

Vertically aligned mesoporous silica [1], with its high surface area and porous structure, serves as an excellent matrix for immobilizing ciprofloxacin and promoting efficient mass transport of analytes. The incorporation of AuNPs within the mesoporous silica provides several advantages, including enhanced charge transfer kinetics, catalytic activity, and increased surface area for analyte adsorption. These properties contribute to improve sensitivity and selectivity of the sensor.

Furthermore, the integration of TiO_2, a wide-bandgap semiconductor material, enhances the photoelectrochemical response of the sensor [2]. Under UV illumination, TiO_2 promotes charge separation and facilitates the generation of reactive oxygen species.

The sensor has been characterized with cyclic voltammetry and electrochemical impedance spectroscopy (EIS). Ciprofloxacin has been detected in chronoamperometry under UV light, thus enhancing the electrochemical signal of the analyte. Also, the sensor's performance in terms of detection limit, linear range, and selectivity for ciprofloxacin detection is thoroughly evaluated, with the potential interference and optimization strategies to improve the sensor's performance in complex sample matrices.

The photoelectrochemical sensor demonstrates excellent performance in detecting ciprofloxacin with high sensitivity and selectivity. The proposed method offers advantages such as simplicity, rapidity, and low-cost compared to conventional detection methods.

[1] M. Etienne, A. Goux, E. Sibottier, and A. Walcarius, *J. Nanosci. Nanotechnol* 9 (2009) 2398-2406
[2] D. Fumagalli, S. Comis, V. Pifferi, and L. Falciola, *ChemElectroChem* 10 (2023) e202201136

OR04

Print-light-synthesis of metal nanoparticles and metal thin film electrodes for electrochemical sensing applications

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The fabrication of metal thin film electrodes and metal nanoparticle (NP)-covered electrodes for electrochemical sensing and energy storage applications by printing techniques is traditionally a two-step process in which i) a metal NP ink, based on previously synthesized NPs, is deposited on a substrate by inkjet- or screen-printing and then ii) thermally treated to obtain films of metal NPs. Herein, we present the one-step fabrication of metal thin films combining drop-on-demand inkjet-printing of metal precursor inks and simultaneous photochemical conversion of the metal precursors into metal NPs. This economic process is known as Print-Light-Synthesis (PLS), which allows large-scale electrode production reducing material waste, fabrication time and costs. Thanks to the high flexibility of the process parameters, thin compact and conductive metallic films can be obtained as well as films of separated metal NPs (Figure 1). Metal precursors, which are present in the ink, are usually metal salts, which are reduced into metals by UV light.

Print-Light-Synthesis has been used for instance for realizing platinum NP-covered electrodes for electrocatalytic applications, such as the Oxygen Evolution Reaction [1]. More recently, PLS gold thin film electrochemical sensors have been used for various analytical applications, such as the detection of alcohols and bacterial infection markers [2]. PLS-Au electrodes showed a higher sensitivity in respect to commercial screen-printed electrodes opening not only new possibilities for large-scale disposable electrode production, but also for improving sensing performances.

We will in particular present various metal-based PLS electrodes for amperometric and potentiometric sensing.

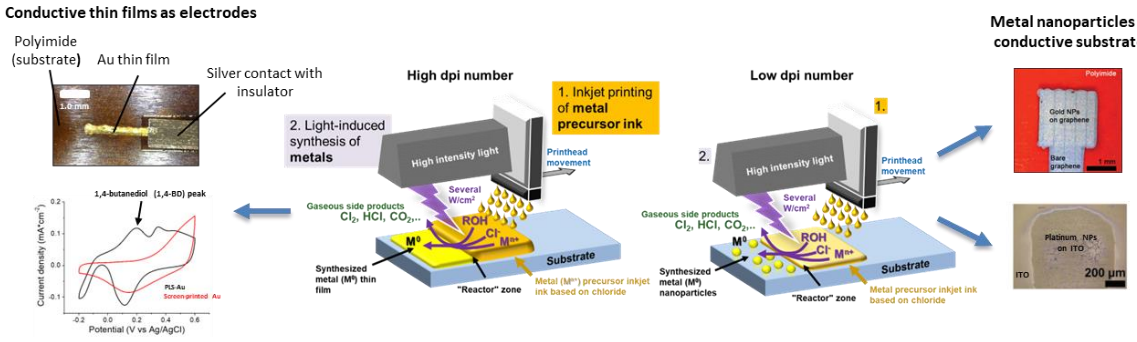

Figure 1: Schematic representation of Print-Light-Synthesis to fabricate compact metallic film electrodes (left panels) and Metal NP coated electrodes (right panels).

[1] A. Lesch, *Adv. Mater. Technol.* 3 (2018) 1–10
[2] E. Maiorano, S. Gianvittorio et al., *Adv. Mater. Technol.* 2202039 (2023) 1–12

OR05

Effect of innovative carbon additives in positive active mass of AGM lead acid battery on dynamic charge acceptance

Marco Cattelan,[a] Marco Mazzucato,[a] Nicola Milani,[a] Mattia Parnigotto,[a] Giorgia Daniel,[b] Daniele Fabris,[b] Silvia Cazzanti,[b] and Christian Durante[a]

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Battery-based energy storage systems with high power/energy densities and excellent cycle efficiencies are expected to play a significant role in our everyday lives. Compared to other energy storage systems, lead-acid batteries (LABs) are often overlooked as an outdated technology with minimal technical potential. Nonetheless, the research on LABs have continued thanks to their properties: stability, reliability, recyclability, and low cost of raw materials. A well-known problem of LABs is the limited charge efficiency and cyclability, due to an important degradation of electrodes during the discharging-charging process. It was observed that small addition (0.5 – 2 wt%) of carbons in the Positive Active Mass (PAM) of LABs improve the battery performances, and specifically the weight, the mechanical strength, and the conductivity which is beneficial for uniform current distribution during the charge-discharge process [1]. A series of carbon-based materials were selected and they were screened on the bases of physicochemical and electrochemical properties such as surface area, porosity, graphitization degree, conductivity, contact angle (wettability), and the overpotential versus the hydrogen evolution reaction [2]. The best candidates were mixed and tested at different loadings in the positive active mass to prepare positive plates from scratch.

A 1+/2– test cell was developed for the electrical, electrochemical, and chemical characterization of the novel electrodes in AGM configurations. The prepared cells were tested under standard charge-discharge protocol and then tested with a homemade protocol for water loss using coupled electrochemical polarization and gas analysis [3] adapted for the AGM configuration in accumulation mode instead of flux mode. The incorporation of carbonaceous materials is evaluated as impact in the charge/discharge performance, in oxygen recombination and plate corrosion of the LAB cell under test, when compared to commercial plates. The effect of increased carbon loading was also considered.

[1] S. Mandal et al., *J. Power Sources* 485 (2021) 229336
[2] B. Marinho et al., *Powder Technol.* 221 (2021) 35
[3] M. Parnigotto et al. *ChemElectroChem* 9 (2022) 20220088

OR06

Towards scaling up in sustainable electrode production

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The maturity of a technology can be well described by the Technology Readiness Level (TRL) scale, to estimate how far a technology is from commercialization. Frith et al. proposed a specific TRL for Li-ion Batteries (LIBs) that highlights the gap between the laboratory studies and the industrial level [1]. This gap is considered one of the most important bottlenecks in the commercialization of new technologies and it is strictly related to the absence of pilot lines at laboratory levels. When cells production is concerned, to scale-up the production process is challenging and it is strongly depending on the chemical composition of the electrode, the interphase with the electrolyte and its composition and the chemical-physical properties of the slurry, which is influenced by the final rheological properties.

The electrode production starts with the mixing of the electrode components (active material, conductive additive, binder and solvent). The used techniques can be very different depending if this is performed at laboratory scale (e.g. magnetic stirrer) or industrial level with bigger slurry amount (e.g. planetary mixer). This technology permits to increase the slurry stability, in particular for water-based production, so avoiding unwanted phenomena such as aggregation and sedimentation, often due to hydrogen bonding. The increase of the solid content of the slurry can limit the sedimentation phenomena, even if it can lead to the increase of the viscosity creating problems during the coating step [2]. The coating is the core step of the electrode production strongly affected by the scale of production: at the laboratory scale, the process is discontinuous while the high yield needed at the industrial level requires a process fully automated and continuous [3]. In particular, at the laboratory level, the main instrument chosen for the deposition is the tape casting (doctor blade), while at the industrial level the technology switch to different types of technologies (slot die coater) [3].

Our research aims to better understand how innovative active materials and aqueous binders perform at different TRL levels to anticipate and propose new solutions to overcome the challenges that the industry will face.

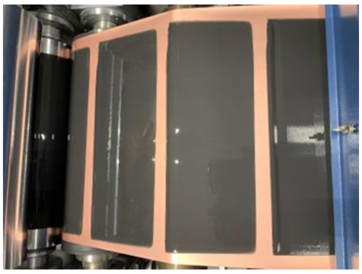

Figure 1: Anode coating on roll-to-roll machine.

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[1] J.T. Frith, M.J. Lacey, and U. Ulissi, *Nature Communications* 14 (2023) 420
[2] W.B. Hawley, and J. Li, *J Energy Storage* 25 (2019)
[3] S.N. Bryntesen, A.H. Strømman, I. Tolstorebrov, P.R. Shearing, J.J. Lamb, and O. Stokke Burheim, *Energies* 14 (2021) 1406

OR07

Dye sensitized solar cells: the role of the electrolytes in the power conversion efficiency under indoor illumination

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The continuous increase in energy demand requires the investigation of renewable energy alternatives. One of the most interesting approaches is the use of photovoltaics. To date, new strategies in solar cell fabrication have been developed with the aim of using both natural sunlight and ambient light (natural and artificial). Such energy can be used to power the numerous devices related to the Internet of Things. For this purpose, dye-sensitized solar cells (DSSCs) can be used.

Compared to other solar cell technologies, they show outstanding performances under indoor conditions with an artificial diffused light source. By using an appropriate dye, thereby taking advantage of scattered light from artificial sources such as light bulbs, DSSCs can generate electricity with significant power conversion efficiencies. To fulfill the green requirements of this type of solar cells, it is mandatory (particularly in domestic applications) to replace the often toxic and volatile organic solvents, typically used in electrolyte solutions, with environmentally friendly solvents, such as Deep Eutectic Solvents (DES). On the other side to increase the performances of DSSCs at low light intensities a new strategy lies in the use of copper complex-based electrolytes which, in the last decades, allowed an increase in the conversion efficiency under indoor illumination.

In this work different combinations of organic dyes, DESs and copper-based electrolyte solutions have been exploited to optimize DSSCs performances under ambient illumination (Figure 1) [1-3].

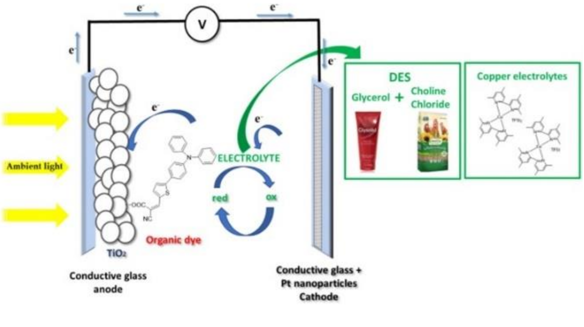

Figure 1: Functional scheme of a DSSC.

[1] C.L Boldrini., A.F. Quivelli, N. Manfredi, V. Capriati, A. Abbotto, *Molecules* 27 (2022) 709
[2] C.L. Boldrini, N. Manfredi, F.M. Perna, V. Trifiletti, V. Capriati, A. Abbotto, *Energy Tchnol.* 5 (2017) 345-353
[3] C.L. Boldrini, N. Manfredi, F.M. Perna, V. Capriati, A. Abbotto, *Chem Eur.J.* 24 (2018) 17656-17659

OR08

Charge-transfer adducts between thiophene derivatives and dihalogens: the role of thiocarbonyl-dihalogen interactions in their supramolecular structure

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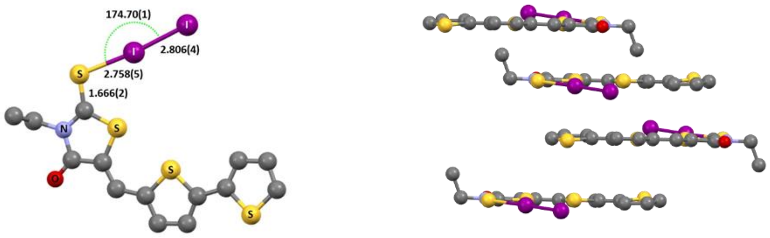
The electronic properties of organic semiconductors (*e.g*. energy levels and optical band-gap) can be tuned by controlling the molecular arrangement of their constituting π-conjugated materials. In this framework, a powerful tool to promote precise solid-state arrangement in semiconductive materials can be offered by crystal engineering [1].

Precisely aimed at advancing fundamental knowledge in the field, we investigated the role of soft···soft interactions between thiocarbonyl donors and molecular halogens. To this scope, representative examples of thiophene-based building blocks functionalized with *N*-substituted rhodanine end-groups have been synthetized and their ability to form crystal structures featuring interactions between the C=S bond and their reactivity towards dihalogens X_2 and interhalogens XY (X, Y = Br, I) investigated. X-ray diffraction and computational studies were performed to characterize the grown crystals. Our preliminary results show that the exocyclic sulphur atom in rhodanine can act as an efficient coordination site for dihalogen molecules through Charge-Transfer (CT) interactions, thus influencing the molecular packing of the thiophene-based compounds [2,3].



(a) (b)

Figure 1: Crystal structure (a) and packing (b) of CT-adduct between a N-ethylrhodanine substituted bithiophene derivative and diiodine.

[1] Y. Le Gal, A. Colas, F. Barrière, V. Dorcet, T. Roisnel, D. Lorcy, *CrystEngComm* 21 (2019) 1934–1939

[2] A. Mancini, L. Pala, M. C. Aragoni, M. Arca, F. A. Devillanova, M. B. Hursthouse, M. E. Light, P. J. Skabara, N. Bricklebank, *Eur. J. Inorg. Chem.* (2012) 2373–2390

[3] M. C. Aragoni, M. Arca, C. Caltagirone, C. Castellano, F. Demartin, P. G. Jones, T. Pivetta, E. Podda, V. Lippolis, S. Murgia, G. Picci, *J. Org. Chem.* 87 (2022) 15448–15465

OR09

Lignin as main precursor of anode and electrolyte for sustainable potassium batteries

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Potassium-ion batteries (PIBs) are one of the top candidates to replace Li-ion batteries (LIBs) for stationary applications. Li-ion batteries have reached unprecedent targets of performance and safety, which ensure the Li-ion system as the best choice for portable devices and electric vehicles. Nevertheless, as lithium is now in the list of critical raw materials due to its low abundancy (0.0017 wt% in the Earth crust), alternatives are coming on the scene. Potassium is abundant on Earth (2.09 wt%), evenly distributed and characterized by a very low standard equilibrium potential and Lewis acidity (smaller solvated ions and, thus, faster conduction). Nonetheless, K-ion batteries have lower volumetric and gravimetric energy density with respect to LIBs, but this makes them perfectly suitable for stationary application. In light of this consideration, it is logical to already design potassium-batteries for large scale commercialization to be sustainable and low cost. Looking at this goal, our groups have carried out the preparation of two main components of this battery (i.e., anode and electrolyte) starting from a widely abundant and sustainable biosourced precursor: lignin.

On one side, we have worked on the design, synthesis and characterization of a lignin-based membrane by crosslinking a pre-oxidized Kraft lignin matrix with poly(ethylene glycol) diglycidyl ether [1]. The polymer electrolyte showed tremendous ability at suppressing the formation of metal dendrites and glorious cycling stability.

In parallel, Kraft lignin was also used as a precursor for the synthesis of a highly porous carbon material to be used as anode material. In particular, after a pre-carbonization process at 250 °C, lignin was mixed with a KOH aqueous solution and urea, and finally activated in tubular furnace at 700 °C under nitrogen flow. Not only the chemical activation requires lower activation temperature, but the resultant material showed a high specific surface area (2900 m^2/g) and very low graphitization degree (i.e., ideal for K-ion insertion). The biobased anode showed an evolving structure that cycle by cycle rearranges itself to accommodate more potassium ions, overall increasing its capacity and cycling stability.

The resulting lignin-based potassium prototype cell is the answer to the quest of an exponentially increasing electrification and large stationary storage demand, but it also fulfills the responsibility for sustainable and low-cost industrial production.

This project has received funding from the European Union's Horizon 2020 Research and Innovation programme (grant agreement No. 952169, project title: SYNERGY).

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OR10

Imidazolium iodide organocatalyst supported on delignified bamboo for the synthesis of cyclic carbonate

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Herein, we report the synthesis of cyclic carbonates from carbon dioxide and epoxides. The reaction is promoted by methyl-1H-imidazol-3-ium iodide which was anchored onto delignified bamboo: a new sustainable and insoluble matrix for recycling. Cyclic carbonates are compounds of great interest for the industry because of their multitude uses such as aprotic solvents for high temperature reaction, electrolytes in batteries, and monomers for the synthesis of polyurethanes and polycarbonates[1].

The hydroxy functional groups on both 1-(2-hydroxyethyl)-3-methyl-1H-imidazol-3-ium iodide and the cellulosic moiety of bamboo were exploited to link them together via new urethane functionalities, by employing HMDI (hexamethyldiisocyanate) as linker.

The immobilization of organocatalyst has been optimized by screen different reaction conditions, and 0.3 mmol/g was the maximum loading achieved. Thus, we tested the catalyst in the carboxylation of styrene oxide by varying temperature and catalyst loading. At this stage we obtained encouraging results (Y = 50 %) by performing the reaction at low catalyst loading (2.8 mol%), 1 atm of CO_2 and moderate temperature (90 °C) in batch operation (Figure 1).

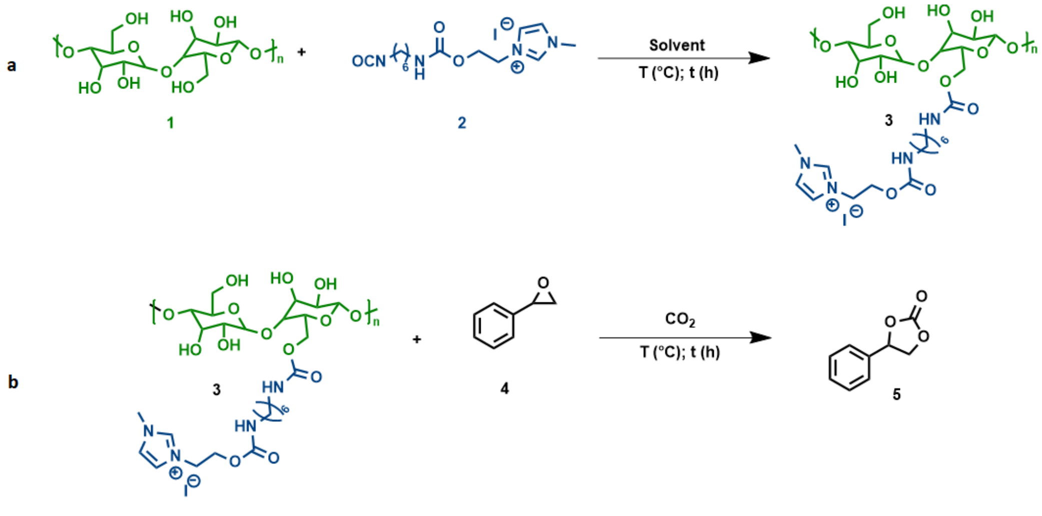

Figure 1. (a) Immobilization of methyl-1H-imidazol-3-ium iodide on natural porous material; (b) cycloaddiction of carbon dioxide to styrene oxide using imidazolium salt supported on natural porous material.

[1] L. Guo, K.J. Lamb, and M. North, *Green Chem.* 23 (2021) 77-118

OR11

Enzymatic route to hybrid prodrugs for the treatment of neurodegenerative diseases

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and Valentina Venturi[b]

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The polypharmacology is a popular approach for multi-target drugs therapy in the form of hybrid molecules. This strategy relies on the use of which integrate multiple pharmacophores through a stable or metabolizable linker [1]. Nowadays, it is widely known that ketone bodies such as acetoacetate (AcAc) exert a protective action against neurological diseases by the control of neuron's oxidative stress and inflammation [2]. Moreover, the ursodeoxycholic acid (UDCA), is a bioactive compound that can cross the blood-brain barrier, displaying therapeutic effects in neurodegenerative disorders [3]. Herein, we describe the enzymatic transesterification of the methyl AcAc with UDCA using various lipases leading to the production of 3α-AcAc-UDCA, 7α-AcAc-UDCA and 3α,7β-*bis*-AcAc-UDCA. The products are unprecedented in literature and have been purified and fully characterized. As the result, the low-cost *Candida antarctica* lipase B, Lipura® Flex affords the best results giving a 67% of UDCA conversion with yields of 25%, 17% and 25% for the products 3α-AcAc-UDCA, 7α-AcAc-UDCA and 3α,7β-*bis*-AcAc-UDCA, respectively.

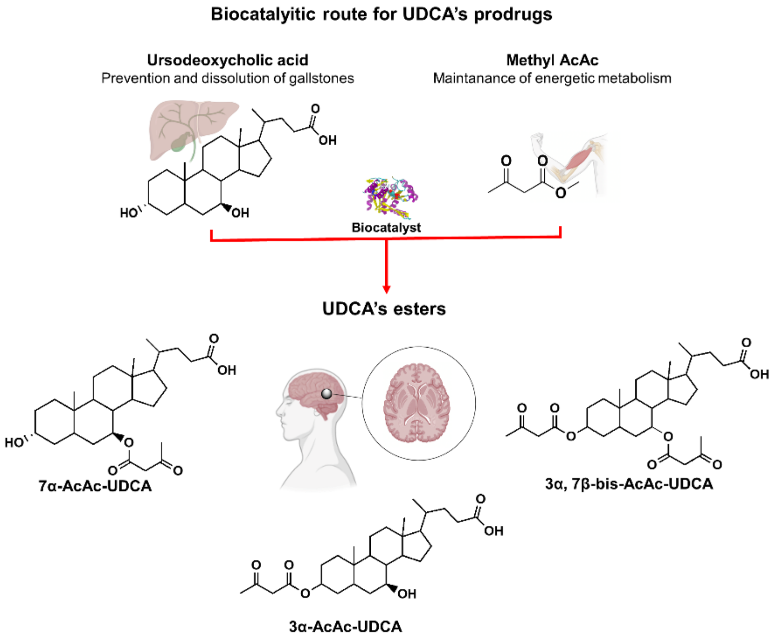

Figure 1: Schematic representation of the enzymatic synthesis of UDCA's esters.

[1] Shaveta et al., *Eur. J. Med. Chem*. 124 (2016) 500-536
[2] Puchalska and Crawford, *Cell Metab*. 25 (2017), 262-284
[3] Amaral et al., *J. Lipid Res*. 50 (2009) 1721-1734

OR12

One-pot enantioselective synthesis of biological active α-amino esters by organocatalysis

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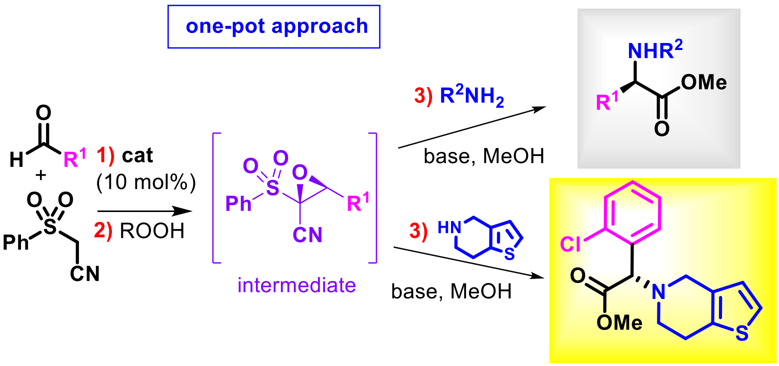
Non-natural aminoacids and in particular α-aryl glycines have been found in an increasing number of bioactive compounds and are precursors of important compounds such as α-amino alcohol. Several synthetic methods have been developed to prepare chiral α-aryl glycines, including the asymmetric Strecker reaction, metal catalysed hydrogenation of α-iminoester as the most investigated. We have recently disclosed a one-pot organocatalytic approach involving new optically enriched epoxides, namely 1-phenylsulfonyl-1-cyano epoxides, useful intermediates to in situ undergo domino ring-opening cyclization (DROC) to enantioenriched dihydroquinoxalinones [1].

In this contribution, we illustrate the application of the same strategy to conveniently access optically active α-aryl glycines and α-alkyl amino esters in good to high overall yield and ee values, starting from commercially available aldehydes, anilines and readily available organocatalysts [2]. A Knoevenagel/asymmetric epoxidation/domino ring-opening esterification (DROE) sequence has been used to conveniently access the enantioenriched products. Moreover, exploiting the same one-pot strategy, a new catalytic preparation of (*S*)-Clopidrogel [3], marketed under the trade name of Plavix, one of the most selling drugs in the world, useful as potent antithrombotic and antiplatelet agent, has been developed (Figure 1).



(*S*)-clopidrogel

Figure 1: One-pot catalytic approach for the enantioselective synthesis of non-natural α-aminoacid esters.

[1] C. Volpe, S. Meninno, C. Crescenzi, M. Mancinelli, A. Mazzanti, and A. Lattanzi, *Angew.Chem.Int.Ed.* 60 (2021) 23819-23826
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[3] A. Saeed, D. Shahzad, M. Faisal, F. A. Larik, H. R. El-Seedi, and P. A. Channar, *Chirality* 29 (2017) 684-707

OR13

New composite HER catalyst obtained by a green fast synthesis to advance alkaline electrolyzers

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Water electrolysis is a leading and promising method in global decarbonization efforts, providing sustainable and fossil fuel-independent approach for hydrogen production. In the pursuit of economically viable water electrolysis implementation, a fundamental requirement is the development of highly active and stable electrocatalysts that avoid the use of critical raw materials. In recent years, transition metal dichalcogenides (TMDs) have gained intensive attention due to their fascinating structure, catalytic properties, chemical stability, and low cost [1]. Currently, the most extensively studied TMD for the hydrogen evolution reaction is MoS_2. However, there is ongoing development and research aimed at discovering promising, stable, and platinum group metal-free catalysts in alkaline electrolytes.

Since it is well known that the nanostructuring of MoS_2 enhances the concentration of catalytically active edges [2], in this work a green and fast method is used to synthesized 2D-MoS_2 on different carbon supports (commercial and S, N-doped). The morphology of the samples was observed by TEM (Figure 1) confirming that MoS_2 nanosheets are obtained and grown well dispersed onto carbon.

The research aims to investigate the synergistic enhancement of HER activities resulting from the presence or absence of heteroatoms within the carbonaceous supports. The activity comparison between commercial, pure and supported MoS_2 is shown in Figure 1.

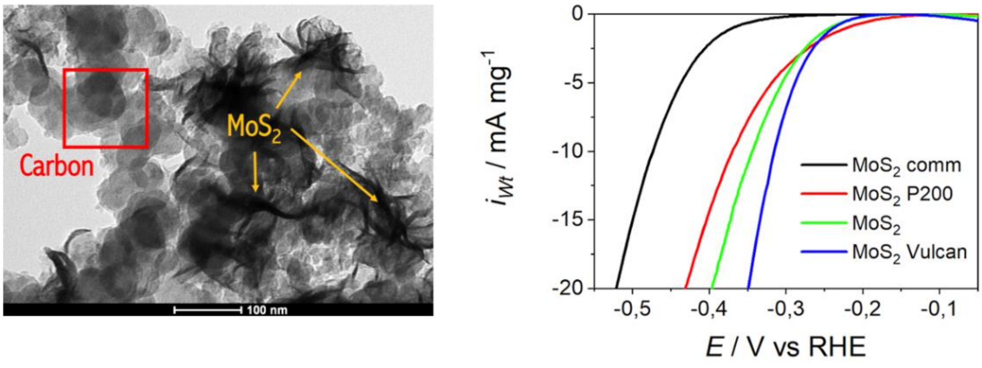

Figure 1: On the left, TEM image of MoS_2 grown on commercial carbon. On the right, HER polarization curves in alkaline electrolyte (KOH 0.1 M).

[1] X. Zou, Y and Zhang, *Chem. Soc. Rev.* 44 (2015) 5148-5180
[2] X. Qian, J. Ding, J. Zhang, Y. Zhang, Y. Wang, E. Kan, X. Wang and J. Zhu, *Nanoscale* 10 (2018) 1766-1773

OR14

Silk Fibroin as a suitable support for heterogeneous catalysis

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Silk fibroin (SF) is an outstanding biopolymer readily available from the cocoons of domesticated *Bombyx mori* silkworms. SF has attracted increasing interest for its different applications, particularly in materials science. Its structure, composed of hydrophobic β-sheet crystalline units alternating with hydrophilic disordered regions [1], gives SF stiffness and mechanical strength, while offering wide opportunities for doping and demonstrating good biocompatibility. SF fibers have been used as inert support for heterogeneous catalysis, due to its chemical stability, high temperature resistance and highly hydrophilic structure [2].

In this work, a SF-Palladium catalyst was prepared and optimized for Suzuki-Miyaura cross-coupling reactions: the desired pure biaryl product was obtained quantitatively under mild conditions, avoiding tedious purification steps and chromatography techniques [3]. Pd/SF was also suitable for gram-scale reactions and for the synthesis of an important pharmaceutical intermediate. It is worth emphasizing that Pd/SF showed an exceptionally high recyclability (up to 19 cycles). Moreover, it has been demonstrated that Pd/SF exhibits a purely heterogeneous catalytic mechanism with no metal leaching during the reactions.

Figure 1: From raw to Palladium supported silk fibroin catalyst for Suzuki-Miyaura cross-coupling reactions.

[1] C. Z. Zhou, F. Confalonieri, M. Jacquet, R. Perasso, Z. Li and J. Janin, *Proteins: Struct. Funct.* 44 (2001) 119-122
[2] A. Akamatsu, Y. Izumi, *Nature*, 34 (1961) 1067
[3] G. Rizzo, G. Albano, M. Lo Presti, A. Milella, F. G. Omenetto and G. M. Farinola *Eur. J. Org. Chem.* 45 (2020) 6992-6996

OR15

Discovery and characterization of a new selective HDAC6 inhibitor against triple negative breast cancer

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Breast cancer (BC) is the most spread cancer type in females worldwide and the most aggressive BC subtype, due to its invasiveness and chemotherapies ineffectiveness, with about one year life expectancy. Triple negative breast cancer (TNBC) cells show uncontrolled matrix remodeling and the consequent epithelial-mesenchymal transition (EMT), which in turn prompt dysregulated invasiveness, proliferation, and differentiation. Recent studies pointed out the role of epigenetic players in TNBC insurgence and progression [1], underlying the effectiveness of targeting histone deacetylases (HDACs) against TNBC tumorigenesis [2]. We recently discovered a novel class of spirocyclic compounds behaving as a potent and selective HDAC6 inhibitors, showing efficacy against TNBC. In particular, compound **1** was assessed in the MDA-MB-231 TNBC cell line showing anti-proliferative effect in MTT assay, related to the activation of apoptotic process. Cytofluorometric assay confirmed the induction of the apoptosis with no effects on necrosis pathways. These data were further validated by western blot analysis, with the detection of cleaved caspase-3, a reliable marker for apoptotic process. Furthermore, increased levels of both Beclin-1 (BECN1) and Bcl-2 interacting protein 3 (BNIP1) were observed after 24 hours of treatment with compound **1**, thus also suggesting the involvement of autophagy process in cell death induction. These results confirm the epigenetic role of HDAC6 enzyme in TNBC tumorigenesis and cancer progression, encouraging the development of new combinatory therapies to assist classical chemotherapeutic approaches.

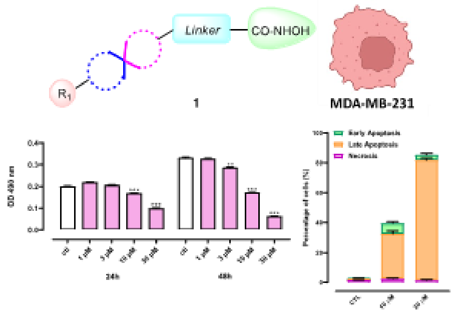

Figure 1: MDA-MB-23 TNBC induced apoptosis after 24 and 48 hours of treatment with compound **1**.

[1] V. Zolota, V. Tzelepi, Z. Piperigkou, H. Kourea, Z. Papakonstantinou, M.I. Artenou, and N.K. Karamanos, *Cancers (Basel)* 13 (2021)
[2] C. Maccallini, A. Ammazzalorso, B. De Filippis, M. Fantacuzzi, L. Giampietro, R. Amoroso, *Pharmaceuticals (Basel).* 15 (2022) 667

OR16

Discovery of NDM-1 non-conventional degraders with a novel mechanism of action to fight antibiotic resistance

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One of the most common mechanisms of bacteria resistance to antibiotics is the hydrolysis of β-lactam antibiotics, which is catalyzed by β-lactamases [1]. The rapid worldwide spread of New Delhi Metallo-β-lactamase-1 (NDM-1) is causing an increased alarm within the scientific community due to its broad spectrum of action, selection of variants, and transferability, representing the highest risk of a new bacterial pandemic [2]. Although various Serine-β-lactamases mechanism-based inhibitors are currently available in therapy, there are no specific and effective inhibitors against NDM-1 in clinical practice [2]. Therefore, there is an urgent need to identify clinically useful inhibitors of Metallo-β-lactamases (MBLs) to be co-administered with existing β-lactams to restore their antibacterial activity. To tackle this rising issue, we used the Pharmacological Protein Inactivation by Folding Intermediate Targeting (PPI-FIT) technology [3] to identify NDM-1 non-conventional degraders. PPI-FIT is a novel and advanced drug discovery approach based on the rationale of negatively regulating protein levels by targeting folding intermediates. Using this approach, we identified NDM-1 putative druggable pockets in a relevant folding intermediate, not present in the native conformation and different from the catalytic site. A structure-based virtual screening was performed, leading to the identification of virtual hits. Here, we report our rationale based on a combined program of medicinal chemistry, structural biology, biochemical testing, and microbiological profiling to identify novel NDM-1 non-conventional degraders.

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OR17

Exploring chemistry-bioactivity of Ru(II)-based metallacycles

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Metal based therapeutics represent a crucial class of antineoplastic drugs, playing a vital role in therapeutic applications. Recently, Ruthenium compounds have been investigated as less toxic and highly promising alternative due to lack of selectivity shown by the ubiquitous Pt-based anticancer remedies that are adverse against normal cells and develop long lasting chemoresistance. The potency of Ruthenium metal drugs extends beyond the cancer treatment, encompassing the development of antivirals, antibiotics, or anti-parasitic agents [1].

Complexation studies of Ru(II) metal centre with several categories of ligands ranging from NSAIDs, pyrroles, indoles, hydroxy stearic acids [2], imines, amino acids to nucleobases have been run aiming to exploit the chemistry with the support of computational studies. The ligands bearing oxygen or nitrogen donor heteroatoms are exemplified by O,O-, N,O- or N,N- bidentate fashion modes. Heterobimetallic complexes based on Ru(II) and Au(I) have been synthesized to further evaluate a synergistic effect towards biological targets. The structures of the novel Ru(II) complexes have been fully characterized by using single crystal X-ray diffraction, ESI-MS, NMR and IR analyses. Biological activities have been investigated as antibacterial tests. Further, detailed information concerning anticancer properties of the complexes have been inferred through the antiproliferative tests on human cancer cell lines.

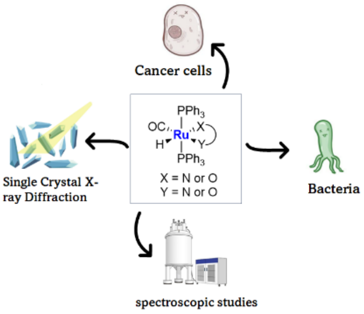

Figure 1: Design and application of the novel Ru(II) species.

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OR18

Detection of hexavalent chromium with nanoscale assemblies

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Contamination of soil and groundwater is one of the major environmental concerns. Chromium in the form of Cr(III) and Cr(VI) is one of the most abundant heavy metals in water. While Cr(III) to some extent represents a micronutrient for living beings, Cr(VI) can cross the plasmatic membrane and damage the DNA of cells [1].

Analytical techniques, such as atomic absorption spectroscopy and mass spectrometry [2], have been used for chromium detection. These costly methods required trained users. The development of smart materials, which allow a fast and selective response to Cr(VI) ions, is of great importance and could be used in remote areas and developing countries.

In this work, a nanoscale assembly consisting of osmium polypyridyl complexes was used to enable ppm-level detection of Cr(VI) ions by naked-eye. The assembly was obtained by spin-coating layers of redox-active osmium complexes on fluorine-doped tin oxide (FTO) on glass. The optical characteristics of the material depend on the oxidation state of the metal ion; while assemblies consisting of Os(II) complexes are brown, the oxidized form, Os(III), appears transparent. Os(II) can be oxidized to its trivalent state by Cr(VI). Concurrently, Cr(VI) is reduced to Cr(III). Immersing the brown nanoscale assembly for a few minutes in a Cr(VI) solution results in a transparent film. The assembly can be reset and reused by washing it with water [3].

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OR19

New rivastigmine-like compounds for the potential treatment of Alzheimer's disease: a multi-target approach

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Alzheimer's disease (AD) is the most common neurodegenerative disorder. Due to its probable multifactorial nature, researchers have focused on the study of multi-target therapeutic agents [1].

Recently, various aryloxyacetic acids were condensed with a fragment mimicking donepezil, an inhibitor of acetylcholinesterase (AChE) used as anti-AD drug [2]. In this new work of the group, the same fragment-based approach to multi-target drug design was used for a new series of hybrids, in which the best aryloxy portions were condensed with a portion mimicking rivastigmine, another drug used in AD therapy as a cholinesterase inhibitor [3]. These structures differ on this moiety for the position of the carbamate on the phenyl group and the alkyl substituents of its nitrogen atom (Figure 1).

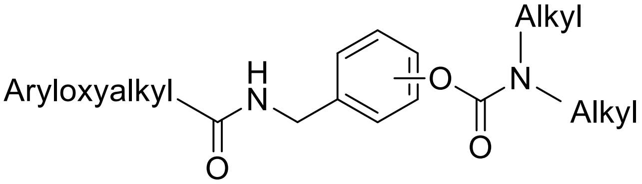

Figure 1: General structure of rivastigmine structure-based hybrids.

Compounds were subsequently assayed *in vitro* as inhibitors of enzymes AChE, BChE (butyrylcholinesterase) and FAAH (Fatty Acid Amide Hydrolase). Some of them were also tested against MAOs (monoamino oxidases), another target for the treatment of AD [3]. Moreover, pharmacokinetic properties of all compounds were predicted *in silico* and also evaluated by analytical methods for most of them.

Preliminary results highlight that these new hybrids based on the structure of rivastigmine could be promising multi-target agents for the therapy of AD. In particular, several compounds of this series showed a good activity up to four of the five tested targets.

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OR20

Moment analysis for predicting separation efficiency in liquid chromatography employing hierarchical pore-structure

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We present a novel homogenization technique that offers a significantly improved speed and accuracy in solving the general advection-diffusion equation within hierarchical porous media [1]. This method specifically addresses localized diffusion and adsorption/desorption processes, thereby enhancing our understanding of the band broadening phenomenon in chromatographic systems [2]. By employing a robust and efficient moment-based approach, we are able to compute precise local and integral concentration moments, enabling exact solutions for the effective velocity and dispersion coefficients of migrating solute particles.

One notable aspect of our proposed method is its ability to capture their entire transient behavior, allowing to identify the necessary time and length scales required to achieve macro-transport conditions accurately. When the hierarchical porous media can be represented as a periodically repeating unit lattice cell (Figure 1A), our method only necessitates solving time-dependent advection-diffusion equations for the zeroth order and first-order exact local moments within the unit cell. Consequently, this approach significantly reduces computational efforts while improving result accuracy compared to direct numerical simulation (DNS) methods that typically require longer flow domains to reach steady-state conditions, often spanning tens to hundreds of unit cells. To validate the reliability of our proposed method, we compare its predictions with DNS results in one, two, and three dimensions, considering both transient and asymptotic conditions (Figure 1B).

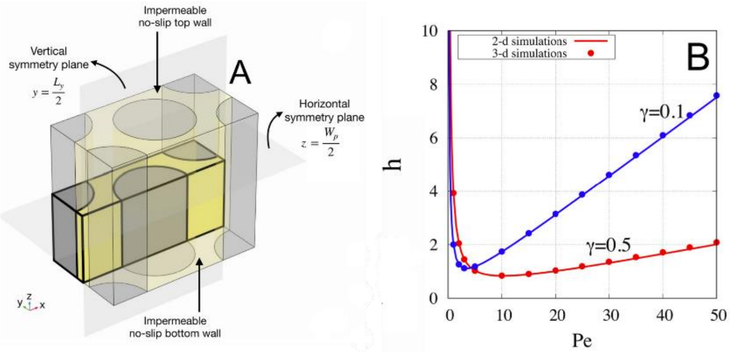

Figure 1: Panel A) 3-d unit cell of the porous pillar array column with macro-porosity ε=0.4. Panel B) Porous-pillar array column. Comparison between 2-d and 3-d results for h vs Pe for k= 2 and D_s=γ D_m with γ=0.1, 0.5.

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OR21

Hybrid hydrogels based on 2D MoS_2 for applications in wearable devices

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The continuous research on electronics, biocompatible materials and nanomaterials has led to the design of a new generation of wearable devices that can be employed in direct contact with the body of the user, which is attractive for real-time, non-invasive health monitoring [1]. For the satisfaction of such requirements, hydrogel-based conductive devices are often proposed as promising candidates for these applications, thanks to their softness, flexibility, and biocompatibility. Here we report the synthesis of conductive hybrid hydrogels containing two-dimensional (2D) MoS_2. The nanoflakes are integrated in the polymeric matrix creating an anisotropic structure, which helps to generate mismatch stress for a strain sensing under a certain stimulus [2], thus allowing the gel to give an electrical response to pressure. 2D MoS_2 nanoflakes were produced via top-down chemical exfoliation [3] and were incorporated in the hydrogel through a covalent grafting to the polymeric building blocks by exploiting the prior surface functionalization of the flakes. The conductivity of the hydrogels was increased with the further incorporation of in-situ polyaniline (PANI), which is a widely used material in biomedical applications as a biocompatible conductive polymer. The as-obtained hydrogels are characterized through a combination of techniques, whereas their electromechanical properties are investigated to prove that compression causes an increase in current due to the piezoresistive properties introduced with the incorporation of 2D MoS_2 and PANI.

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OR22

Stereolithography of bio-scaffolds using bone waste

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Additive manufacturing allows to fabricatate bioscaffolds with precise and personalized design for better integration with bone defect [1]. The most commonly used biomaterial for bone regeneration is hydroxyapatite. It is a major component in human bone composition with excellent biocompatibility, bioactivity and biodegradability. Hydroxyapatite can be synthesized chemically or extracted from natural sources [2].

In this study waste of bone is used as a source of natural hydroxyapatite to additive manufacture bioscaffolds (Figure: 1). It was extracted from bovine through a series of processes, including boiling, defatting, deproteinization, drying, and calcination at 900°C. Natural hydroxyapatite is more suitable for medical applications. It contains carbonate groups and trace elements such as magnesium, sodium, and other metals which are essential for the bone regeneration. Extracted hydroxyapatite was used to prepare UV curable slurries for stereolithography. The slurries are prepared adding different amount of hydroxyapatite to SiO_2 containing ceramic resin. When the concentration of hydroxyapatite is 20% or more, slurry is not printable because of high viscosity.

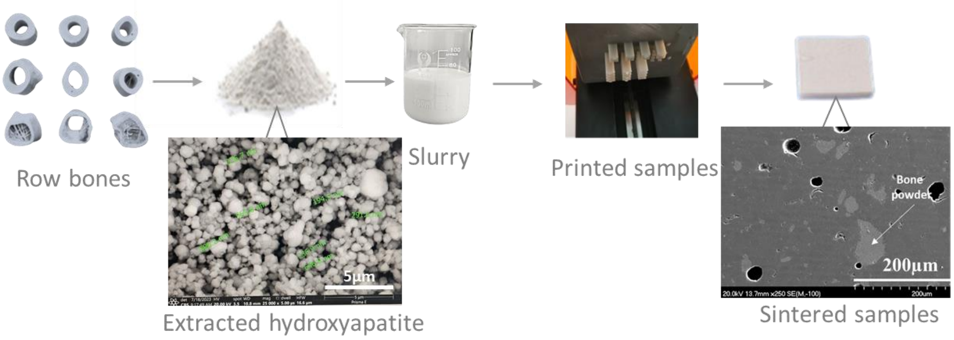

Figure: 1 Scheme of extraction natural hydroxyapatite and fabrication of bioscaffold.

Addition of hydroxyapatite in the slurries leads to a reduction in porosity and enhances the mechanical properties of bioscaffolds. Notably, this results significantly improves compressive and flexural strength.

Cytotoxicity experiments show that the bioscaffolds do not have negative impact to the growth and viability of Wt-19 fibroblast cells. The bioscaffolds exhibited favorable cell attachment properties.

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OR23

Preventing the flip! Investigation of the stereochemical lability of benzo-cycloheptene-based drugs characterized by potentially modulable planar chirality

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Chirality is a common feature in bioactive compounds and a high percentage of the drugs available on the market are often formulated using only a single enantiomer. However, the unfavorable effect deriving from the possible lability of a stereogenic element, possessed by drugs administered as single enantiomers, cannot be overlooked, taking into account the different pharmaceutical activity that these could exhibit. In fact, in the human organism, the manifestation of stereochemical fragility could lead to racemization. With attention focused on this subject, both theoretical and experimental studies were performed to analyze the configurational lability possessed by the enantiomers of some popular second-generation antihistaminic drugs. These molecules are endowed with a central seven-membered benzo-cycloheptene non-planar ring, responsible for the manifested chirality, on which it is connected a 5-ylidenepiperidine moiety. The absence of planarity allows the existence of two enantiomeric species that can interconvert thanks to a ring overturning mechanism. The obtained results have suggested which kind of structural modifications can be rationally designed in order to modulate the intrinsic stereolability, so allowing to suitably increase of the involved enantiomerization barrier [1]. The goals were achieved, starting from the structure of pizotifen (Figure 1) and of some its derivatives, by having recourse to both kinetic (dynamic chromatography and off-column racemization) [2] and theoretical methods, based on DFT molecular modeling calculations, employed in a rigorous and integrated way. This could be a useful approach that can be exploited in a wide variety of situations related to stereolability due to flipping of chiral planes.

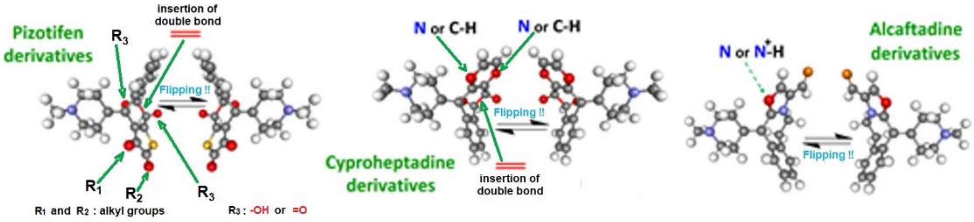

Figure 1: Rational design of structural modifications useful to modulate planar stereolability of chiral drugs.

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OR24

New small nitrogen heterocycles as correctors for the functional rescue of F508del-CFTR in cystic fibrosis

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Cystic fibrosis (CF) is a genetic disease caused by mutations that impair the function of the CFTR chloride channel. This defect can be overcome by CFTR “correctors” that stabilize misfolded protein and increase membrane expression [1-3]. Although significant advances have been obtained by combinations of correctors with complementary mechanism, new modulators are still needed to maximize the rescue F508del and other CFTR mutants with trafficking defects. In the course of our studies, we have identified a new class of small molecules (PP compounds), as correctors with high efficacy in the rescue of F508del-CFTR on native epithelial cells of CF patients particularly in combination with class 1 correctors (VX-809).

The synthesis of nearly 300 derivatives gave an insight of the structure-activity relationship of these molecules as CFTR correctors. A multiparametric optimization of PP compounds is ongoing to generate new candidates with improved features, either in terms of corrector potency/efficacy and drug-likeness.

The new compounds are tested functionally on cells with stable expression of mutant CFTR and the halide-sensitive yellow fluorescent protein (HS-YFP). The most active compounds are then validated: i) in short-circuit recordings on primary airway epithelial cells (bronchial and/or nasal); ii) in biochemical and microscopy assays to evaluate CFTR maturation/trafficking.

Iterative cycles of chemical synthesis have led, so far, to new derivatives clustered into: 1) analogues of the parent core; 2) new chemical scaffolds based on a free rotable structure. For many compounds, a rescue comparable to that of VX-809 was found. Furthermore, the evaluation of corrector activity indicated that PP compounds act as class 3 correctors, since they induce synergistic effect when combined with class 1 (VX-809) and 2 (3151) correctors but not with class 3 (4172).

We have identified novel CFTR correctors, with promising features for the development of combinatorial treatments for CF. The optimization process is ongoing, in order to obtain the best trade-off between potency/efficacy and “drug-likeness” to develop an optimized lead compound that could be considered for preclinical and clinical development.

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OR25

Development of novel SR ligands with antiallodynic effect

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Pain is a serious health problem affecting the life of million people in the world, with significant costs on the healthcare system. In many cases, current analgesics provide only modest efficacy being limited by a number of side effects. As part of our research program aiming at the discovery of novel sigma receptors (SRs), here we report on the synthesis and biological evaluation of a library of SR ligands based on 2,7-diazaspiro[4.4]nonane scaffold. After determination of affinity toward S1R and S2R in radioligand binding assays, molecular modeling studies were carried out to deeply analyze the binding pose. The iterative optimization has been developed according to structure-affinity relationships approach consisting of (i) design of new candidate ligands, (ii) in vitro radioligand binding assays, (iii) iterative compounds design based on affinity and selectivity, (iv) computational studies, (v) synthesis of the new compounds for further pharmacological evaluation. The most notable compounds have been subjected to in vitro toxicity evaluation and subjected to dose-dependent antiallodynic effects against capsaicin-induced pain in mice. Among these, compound 9d emerges for its potent antiallodynic effects with a dose able to fully reverse mechanical hypersensitivity of 1.25 mg/Kg making this compound one the most potent S1R antagonist reported so far.

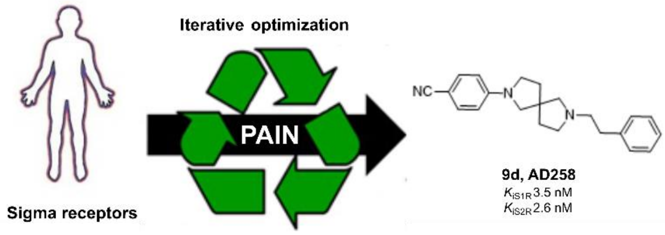

Figure 1: Development of compound 9d.

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OR26

Development of a novel library of 3-amino-1,2,4-triazine compounds as PDK inhibitors: synthesis, biological evaluation, and structural manipulation

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Recently, the hybridization approach, which combines different pharmacophoric moieties in a single structure, has gained particular interest in developing novel small molecules endowed with several biological effects, including anticancer [1].

Among the various pharmacophoric groups, nitrogen heterocycles, stand out due to their ability to form hydrogen bonds with the ATP binding pocket of protein kinases and other significant electrostatic interactions crucial for kinases inhibition. Specifically, analyzing different promising 5- or 6-membered nitrogen heteroaromatic fragment kinase hits; triazines, indoles and azaindoles, were highlighted as versatile scaffolds for developing small molecules kinase inhibitors [2,3].

Considering these factors, herein we report the synthesis and biological evaluation of new 3-amino-1,2,4-triazine hybrid compounds.

The ability of derivatives to inhibit cancer cell growth in highly resistant pancreatic ductal adenocarcinoma (PDAC) was assessed in 2D and 3D cancer cell models. All compounds exhibited a very promising antiproliferative activity, with IC_{50} values ranging from low- to sub-micromolar level.

Furthermore, the potential of triazine derivatives to interfere with the function of proteins involved in PDAC progression and resistance, such as pyruvate dehydrogenase kinases (PDKs) enzymes, was tested. The results, showed a strong reduction in PDK1 catalytic activity, exhibiting IC_{50} values ranging from 0.01 to 0.33 μM, significantly more potent than the well-known PDK1 reference inhibitor, dichloroacetate (DCA). Preliminary *in vivo* studies were also performed on the best derivatives to validate their antitumor potential, highlighting an equal efficacy and a better tolerability profile with respect to reference FDA approved drugs, cisplatin and gemcitabine.

As a proof-of-concept, further studies to confirm the ability of the new library to act as PDK1 inhibitors, will be presented and discussed.

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OR27

Integrative biophysical approach based on NMR, SAXS and MS to unravel the structural properties of the OSCP subunit of the ATP synthase

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The Permeability Transition Pore (PTP) is a Ca^{2+} -triggered channel, detected in the inner mitochondrial membrane, whose opening leads to cellular death through apoptosis [1]. PTP dysregulated activity is directly related to aging and several human diseases as Alzheimer's and cancer. Even though the molecular structure of PTP has not been fully elucidated, experimental evidences indicate that ATP synthase is most likely the PTP main component.

The ATP synthase subunit OSCP (Oligomycin Sensitivity Conferral Protein) is an emerging therapeutic target for its putative role as the molecular switch for the regulation of PTP. In fact, OSCP is the binding site for Cyclophilin D (CypD), the immunomodulatory benzodiazepine Bz423 and the mitochondrial inhibitor IF1 [2] which are three PTP modulators. Targeting the OSCP to achieve a drug-based control of the PTP opening represents an interesting therapeutic perspective. A huge limit in this sense is made by the possibility to manage the isolated OSCP in solution. Unfortunately, OSCP is described to be very prone to non-specific aggregation when it is disconnected from the rest of the ATP synthase, as well as its C-terminal domain OSCP-CT [3]. Only the N-terminal domain of the protein was obtained in solution and then characterized by NMR spectroscopy [3].

Here we report the first biophysical characterization of both OSCP-CT and OSCP subunit in solution, due to the synergic use of NMR spectroscopy, Small Angle X-ray Scattering (SAXS) and native Mass Spectrometry (MS). Unlike that reported in literature, we obtained the recombinant C-terminal domain and the full protein through pET SUMO expression strategy. In this way, we found that both protein constructs do not aggregate in solution but they are involved in an unexpected oligomerization equilibrium in which the monomeric state seems to be not highly populated. We therefore designed and synthetized a peptide for stabilizing the monomeric OSCP-CT as well as the full protein. Overall, our results make the OSCP suitable for further interactions studies in solution, with both novel and old interactors. Our work will help to strengthen the role of OSCP as the first protein target for the regulation of PTP activity.

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OR28

Carbon nanodots as versatile linkers between molecular and nanoscale worlds

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Carbon nanodots (CNDs) are defined as carbon nanoparticles with size below 10 nm which possess intriguing properties like tunable light-emission and rich-surface chemistry [1]. The commonly employed synthetic strategy for the preparation of these materials relies on the solvothermal treatment of small organic molecules. In recent years, our group have contributed to the development of reliable synthetic and purification strategies for the preparation of these nanoparticles, exploiting combined characterization techniques to study their purity and composition [2]. Leveraging on our expertise, we have recently synthesized a new type of chiral CNDs. The so-obtained chiral materials were exploited to promote photo-organocatalytic transformations enabling the use of these particles as metal-free nano-catalytic platform [3]. As final goal, we moved from the synthesis of individual CNDs to their assembly into larger systems, paving the way for the organization of these materials across multiple length scales. This talk aims to present the unique and adaptable features of CNDs which stand as versatile linkers between molecular and nanoscale realms.

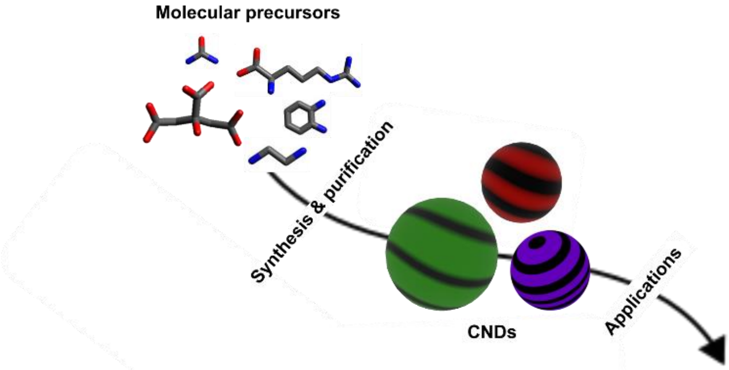

Figure 1: General representation for the synthesis and applications of CNDs.

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OR29

Halloysite – protoporphyrin IX a promising nanomaterial for potential photodynamic therapy

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The porphyrins are an important class of naturally fluorescent occurring macrocyclic that play a very important role in the metabolism of living organisms. From a biological point of view, porphyrins can be used as photosensitizers for photodynamic therapy (PDT). However, porphyrins show several disadvantages, such as low water solubility, cutaneous photosensitivity, and reduced selectivity for targeted tissues which hampered their clinical use.

Halloysite is an aluminosilicate clay belonging to the kaolin group with a typical hollow tubular structure and dimensions in the nanometric range (HNTs). Halloysite nanotubes are biocompatible, available in large amounts at low cost, capable to penetrate the cellular membranes, localizing themselves in the perinuclear region. In the last years, the modification of HNTs with different biological active species allowed to synthetize valuable carrier and delivery systems.[1]

Herein we report studies about the covalent modification of halloysite nanotubes with protoporphyrin IX (PPIX) to develop potential systems for PDT. The obtained HNTs-PPIX nanomaterial was used as chelating agent for bivalent ions such as cobalt, zinc, and copper. The photoluminescent properties of HNTs-PPIX was also investigated and, PDT analysis was studied by the generation of ROS by using 1,3-diphenylisobenzofuran (DPBF) as a singlet oxygen scavenger under irradiation.

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OR30

Small amphiphilic peptides behave as efficient hydrogelators

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Low molecular weight gelators (LMWGs) are small molecules that form gels with many desirable properties making them useful in various fields including applications as drug delivery carriers [1]. Among them, peptide-based gelators are very efficient and versatile molecules as they self-assemble into layered structures to form gel networks. Therefore, their formation and disruption can be easily controlled. Also, they consist of eco-friendly amino acids, which makes them biocompatible and easily biodegradable.

In order to further understand the relationship between gelator structure and gelation attitude, we designed and synthesized a library of eighteen peptide-based gelators, coupling amino acids (phenylalanine, tyrosine and 3,4-dihydroxyphenylalanine). Most of them were found to be gelators in aqueous environment at concentrations lower than 1% w/v. Moreover, a few of them rendered remarkably stable gels in aqueous solutions at concentrations below 0.5% w/v and one gelator satisfied the gelation requirements to be defined a super gelator.

The investigation of the self-assembly process of such peptide with different alkyl chains can give further insight into the dynamics of formation of various supramolecular structures.

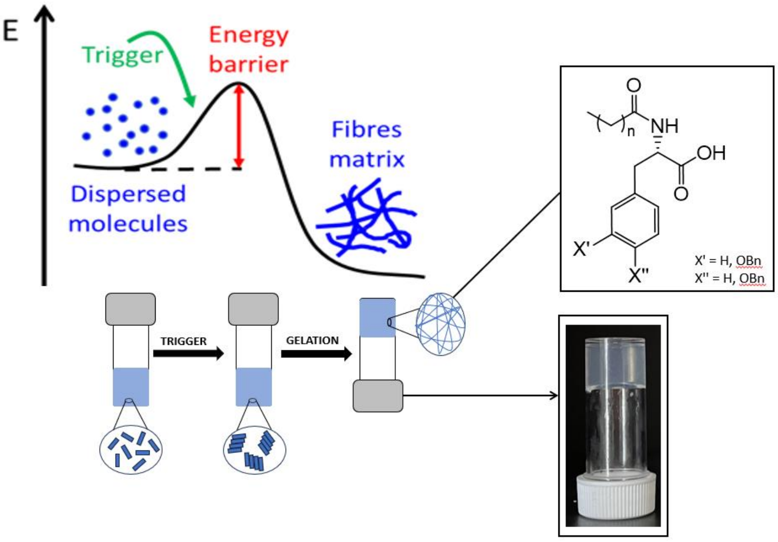

Figure 1: Representation of the fibrous network's formation.

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OR31

Naproxen drug delivery through artificial human epidermis by functionalized diatoms biosilica

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Nanostructured silica-based materials are of great interest thanks to their structural porosity, high surface area, biocompatibility and the possibility of chemical modifications [1]. Diatoms microalgae represent a natural reservoir (both *in vivo* and as fossil sediments) of nanostructured biosilica microparticles. Although biosilica has been already tested for drug delivery systems [2], their skin application was tested for the first time in this work. Biosilica microparticles were chemically modified with n-octyl-triethoxysilyl groups to obtain a hydrophobic material that can stick to human skin, interacting with the lipidic matrix of this organ. After characterization, Naproxen was selected as a model drug to test. In vitro experiments of drug release were performed both in an artificial sweat solution and by transepidermal drug permeation through a 3D living skin tissue. Cell viability and morphology after transepithelial permeation showed no significant cytotoxicity effect on human epidermis models for all the tested treatments. Octyl chains were demonstrated to not only favour the microcarriers adhesion onto porcine skin tissues but also to control the gradual release and the transepidermal permeation of Naproxen for 24 hours, disclosing promising applications of these drug-delivery systems for skin diseases therapies.

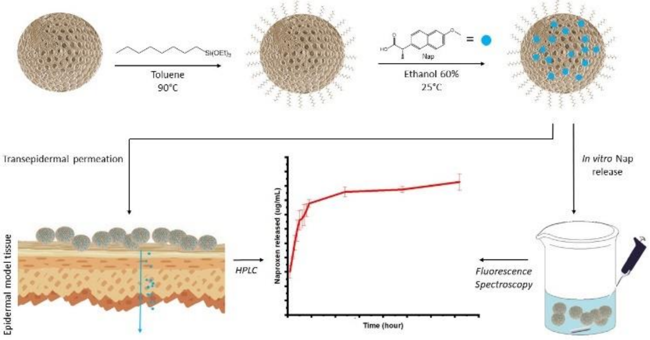

Figure 1: Schematic representation of hydrophobic diatom-based microcarriers loaded with Naproxen and tested for *in vitro* drug release both with artificial human epidermis and artificial sweat solution.

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OR32

N-lactam radicals: light-driven generation and application in APIs synthesis

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We report the synthesis, the photocatalytic activation, and the application in APIs synthesis of a novel class of nitrogen-centred radicals (NCRs): *N*-lactam radicals.

According to their structure, *N*-lactam radicals can be classified as electrophilic Amidyl NCRs, which can be generated by homolytic cleavage of a nitrogen-involving bond, after a single electron transfer (SET) triggered by light [1]. The great potentiality of NCRs is the possibility to be exploited as highly energetic synthetic intermediates, to introduce nitrogen-containing functional groups in complex target molecules, through a completely innovative strategy that relies on the combination of the chemistry of radicals with photocatalysis.

The use of light in chemical transformations has been object of great studies in the last decades, enhancing the efficiency of radical-involving processes. Photochemistry underwent a great growth since it opened the door to the development of greener and more sustainable methods. The possibility to perform challenging reactions under milder conditions, using cheap and safe redox species made photocatalysis an appealing and powerful synthetic tool.

The first goal of this work was the development of an efficient synthetic route for the radical precursor, the *N*-aminopyridinium salt **1**. Taking inspiration from the work of Studer and coworkers, the desired precursor was successfully synthesised on a 10-gram scale, in 48% overall yield, through a five-step synthesis, starting from cheap and commercially available benzophenone hydrazone [2].

Once synthesised the precursor, a light-mediated process was exploited to generate the desired radical. The light-triggered addition of the radical to an electron-rich aromatic ring was the model reaction exploited to fine tune the conditions for the radical generation and it became the opportunity to study its reactivity [2].

Once achieved this result, the reactivity of the *N*-lactam radical was further explored testing a nucleophile of a different nature: the enamine of aldehydes [3]. This reaction was also developed in a stereoselective version, for the application in the synthesis of an API.

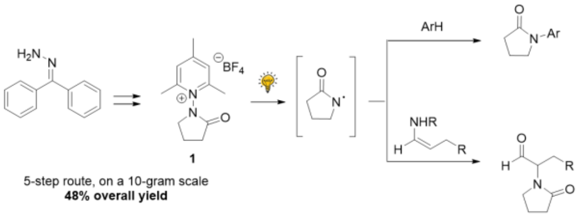

Figure 1: General reactivity

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OR33

A novel photochemical approach to synthetize APIs: the use of nitrogen-centered amidyl radicals

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The chemistry of radicals has developed extensively in recent years. Their appreciation in synthesis is related to the feasibility of few synthetic pathways which could be considered highly challenging or unapproachable if conventional methods are used. The traditional chemistry involves Pd-catalyzed Buchwald-Hartwig amination or Cu-catalyzed Ullman type coupling to form C-N bonds. However, high temperatures and pre-functionalized coupling partners are required to successfully provide the desired results [1]. *N*-centered radicals can be prepared and introduced onto the appropriated substrates under mild conditions *via* photoredox catalysis.

My research work aimed to consider photocatalytically generated *N*-oxazolidinone radicals within the synthesis of different APIs as illustrated in **Figure 1**, a) and b). The development of antibiotic resistance has dramatically increased over the last decades. An efficient strategy against resistant human-pathogenic bacteria was found to be the use of drugs acting as bacterial protein synthesis inhibitors, such as oxazolidinones, which were introduced into the clinic in the 1970s [2]. The toxicity issues of the class were overcome by two nontoxic molecules, linezolid and eperezolid, twenty years later. The SAR studies revealed how the *N*-aryl substituent is one of the essential factors for the pharmacological activity. Here I present some preliminary studies concerning the synthesis of the APIs of **Figure 1**.

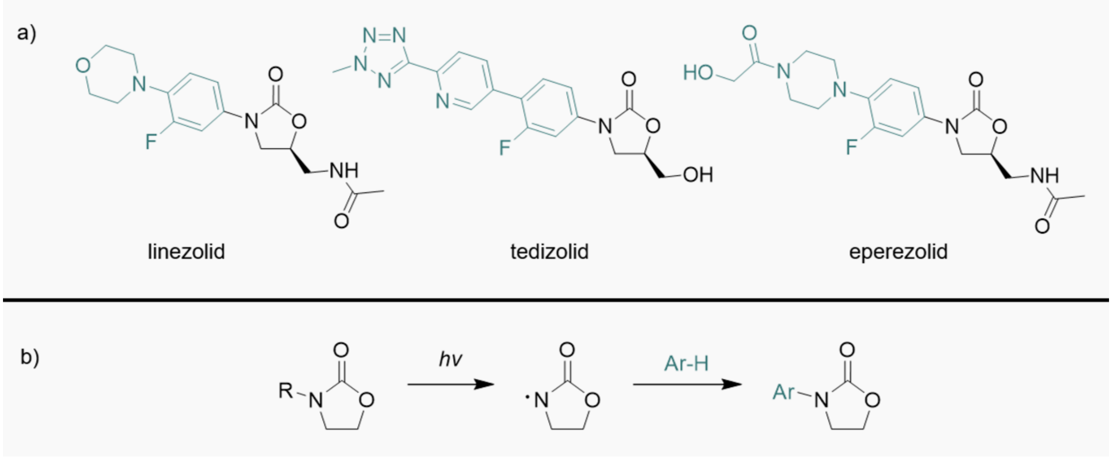

Figure 1: a) Representative chemical structures of APIs and b) synthetic strategy

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OR34

Highly efficient electrochemiluminescence from imidazole based thermally activated delayed fluorescence emitters

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Electrochemiluminescence (ECL) is a process that uses an applied electrical bias to generate reactive species at an electrode surface that undergo subsequent electron-transfer reactions to generate luminescent species. This process could be used to amplify signals of analytes, making this technique the most powerful tool for biomedical applications.

However, due to spin statistics only phosphorescent emitters such as Ru(II) or Ir(III) complexes could be used efficiently to harvest triplet states thanks to the strong spin-orbit coupling which favors intersystem crossing.

To avoid these expensive metal complexes, purely-organic compounds showing the Thermally Activated Delayed Fluorescence (TADF) can be used to harvest triplet excitons [1]. TADF is a phenomenon shown by molecules that possess a tilted donor-acceptor structure where HOMO and LUMO are spatially separated and a small energy gap between S_1 and T_1 states is present. This small energy gap increases the reverse intersystem crossing process enhancing Internal Quantum Efficiency and making these compounds very intriguing for ECL applications.

However, almost all examples about ECL of TADF molecules are performed in the so-called "annihilation way", where compounds are subsequently oxidized and reduced, while there are only few examples of ECL of TADF molecules in presence of a coreactant [2].

Herein we present a family of novel TADF emitters bearing a fixed acceptor moiety, 4-(1H-imidazol-1-yl)benzonitrile, where donors were systematically varied in order to correlate photophysical and electrochemical properties with their performances in electrochemiluminescence in presence of benzoyl peroxide as coreactant [3].

Moreover, the imidazole moiety can be efficiently alkylated with chains bearing functional group, such as tert-butyl esters, enabling practical applications.

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OR35

Charge and Energy Transfer Kinetics in Ternary Organic Solar Cells

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Photovoltaic (PV) represents one of the most important renewable-energy technology. Lately, research efforts have been focused on low-cost solar cells based on organic materials (OSC). Unfortunately, OSC power conversion efficiency (PCE) is still much far from the theoretical Shockley-Queisser limit of 33% for single junction devices and from the efficiency of inorganic devices. This can be imputed to very fast radiative and non-radiative decays to the ground state. In fact, it was the removal of non-radiative decay channels the real breakthrough for achieving high efficiency in GaAs based solar cells[1].

Thus, characterizing the kinetics of all processes is of paramount importance in order to recognize both beneficial and detrimental processes affecting the PCE of OSCs. This task requires the computation of the rates for all charge and energy transfer processes occurring in the device. To that end, we developed a theoretical method for computing the rates (k) based on the Fermi's Golden Rule [2].

We tested our method on the very challenging case of a ternary OSC (TSC). There, the occurrence of several concomitant processes at three different interfaces, strongly complicate things with respect to binary devices. For the TSC composed of FG3, FG4 and Y6, two small molecules donors (FG) and one acceptor [3], we computed the rates of photo-electron transfer (PET), photo-hole transfer (PHT), charge recombination (CR) and Förster resonance energy transfer (FRET) using our newly developed methodology.

We started our study performing MD simulations, since it is widely recognized that the morphology interface deeply influences the rates. The most significant MD configurations were extracted from dynamics and then characterized at the DFT level to compute the electronic couplings for all processes. FCWD was evaluated, introducing the harmonic approximation, by the generating function approach (GF). The GF has indeed several advantages because it permits to take into account all the vibrational modes and also includes thermal effects.

Preliminary results strongly indicate FRET as the most beneficial process and predict an efficiency substantially higher than the one of the binary devices counterparts. In fact, simulations of the OSC obtained by removing one of the donors (thus resorting to the binary device) predict a substantially lower efficiency, in good agreement with experimental results.

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OR36

Innovative green strategies to reduce the chemical oxygen demand in landfill leachate concentrate

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The simple and cheap way for the final disposal of solid waste is landfill. In landfill the main pollutant outputs are biogas and leachate [1]. Landfill leachates are products due to the water percolation through waste deposits and consist in a mixture of highly concentrated organic and inorganic contaminants, which are difficult to be degraded and need to be appropriately treated because of their toxicity and severe adverse effects on the environment. These processes require intense harsh physical and chemical conditions to comply with strict environmental regulations. A fundamental parameter that allows to classify leachate is their Chemical Oxygen Demand (COD), *i.e.* the amount of oxygen required for the oxidation of organic and inorganic compounds present in a water sample, expressed in mg/L [2]. COD allows to evaluate the degree of pollution of landfill leachate. The COD test uses strong oxidants such as $K_2Cr_2O_7$ and H_2O_2 to oxidize the organic matter more effectively with respect to microorganisms. The COD of samples is calculated versus standards such as phthalate. The leachate used in our study is a concentrate obtained from a chemical physical pretreatment, specifically a reverse osmosis process. The concentrate has a COD value of 16000 mg/L and an almost neutral pH (7.3). On this ground, our research aims to define innovative eco-friendly, fast, and cheap strategies for COD reduction and detection in landfill leachate concentrate, with the aim of comparing their performance in the COD reduction with the state of art. The landfill leachate concentrate was subjected to a series of treatments including transition metal catalyzed oxidation reactions and the resulting mixture was subjected to a Gel Permeation Chromatography (GPC) as an innovative detection method of COD, that was compared to the well-known EPA 410.4, revision 2.0 method.

A significant reduction in the chromatographic peak of the organic eluate was observed, demonstrating the effectiveness of our strategy for the treatment of landfill leachate concentrate.

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OR37

Electrochemical chlorination of aromatic compounds: comparison between batch and flow reactions

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Aromatic halides are essential molecules in agrochemical, medicine and advanced materials [1]. The most classical method to synthetize them, is through the electrophilic substitution of aromatic compounds using halogenated sources which are low atom-economy (such as NBS or NCS) or not environmentally friendly (like Br_2 or Cl_2) reagents. Organic electrochemistry is a powerful tool that can be used to overcome these limitations since its application requires greener halogenated sources like alkali metal halides [2]. Even if electrochemical halogenation reactions, especially chlorination ones, have been studied for many years, they still suffer of a limited substrates scope. Indeed, electron-poor systems show less reactivity compared to the electron-rich ones and a possible polymerization of the aromatic compounds affects heavily the product yield [3]

In thise freamwork, we decided to exploit the advantages of the flow chemistry in the electrochemical chlorination of 1,3,5-trimethoxybenzene (**1**) and 1,3-dimethoxybenzene (**2**) as reported in **Figure 1**. The comparison between batch and flow chemistry shows an enhancement of the yields along with the productivity for the in flow process. Further chlorination reactions of aromatic compounds are still in progress and will be presented.

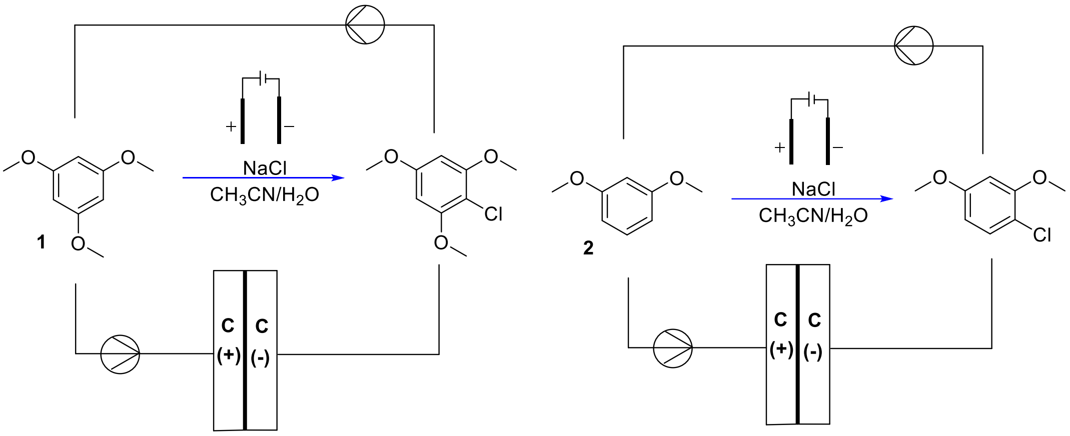

Figure 1: Electrochemical chlorination pathways of compound **1** and **2** in batch (blue) and in flow (black)

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OR38

Upcycling of pomegranate peels: sustainable extraction of metabolites and their antiproliferative and antibacterial activity

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Pomegranate peels (PP), usually discarded during fruit processing, contain a wealth of compounds with various biological activities, including antioxidant, antimicrobial, and anticancer properties. In this work, MW -assisted extraction (MAE) in water to recover metabolites from PP, refining temperature, extraction times and energy consumption are studied. The total phenolics, anthocyanin, flavonoid, and tannin contents of the extract were determined, as well as their antioxidant activity (356.35 mgGAE/gextr, 303.97 µgCy3G/gextr, 37.28 mgQE/gextr, 56.48 mgGAE/gextr, and 1.43 µmolTE/gextr, respectively). In addition, the study investigates water recycling by nanofiltration in the downstream extract. In this way, approximately 75% of the water is recovered (reusable in a new extraction), achieving the desired side effect of product concentration with significant time and energy savings. The overall sustainability of the PP valorisation strategy is evaluated by energy consumption (20.92 W/mgGAE) and other green metrics such as reaction mass efficiency, E-factor and Process Mass Intensity. Finally, the antimicrobial properties of the extracts of PP were evaluated against Gram-positive and Gram-negative bacteria, as well as their antiproliferative activity towards human cancer cells (HeLa). The extracted metabolites resulted extremely effective against *S. aureus* and *P. aeruginosa* bacteria, and also showed dose-dependent antiproliferative activity in HeLa cells, supported by clonogenic analysis for growth inhibition.

The information gathered supports the proposed valorization protocol as an environmentally friendly and sustainable approach for upcycling PP, achieving a final product with interesting biological features.

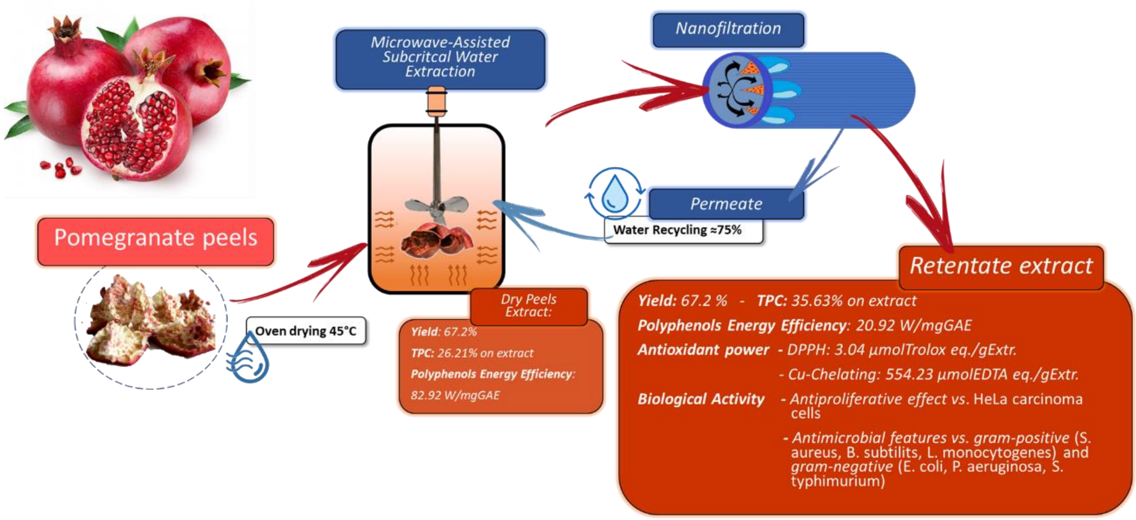

Figure 1: Optimized up-cycling strategy for PP combining MAE and nanofiltration.

OR39

Continuous flow Pd-catalyzed cross-coupling reactions with organolithium

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The present work has as objective the use of flow chemistry to develop a safer, faster and cheaper version of the palladium-catalyzed Murahashi cross-coupling reaction [1], that involves the use of organolithium reagents as nucleophilic coupling partners. Organolithium are more electropositive than other organometallic compounds and this favours the transmetalation step. Another great advantage is that they are commercially available and cheap or can be easily generated.

Feringa and co-workers have improved this reaction and in 2017 have reported a fast cross-coupling reaction using organolithium, thanks to the use of oxygen for the activation of the palladium catalyst [2].

Some problems that chemists may encounter in the scale-up of this reaction in batch are related to inefficient mixing, poor heat transfer and safety problems related to the use of flammable and sensitive to air and moisture compounds. The solution can be the use of flow chemistry, where channels with small dimensions allows a better mixing and a better heat transfer.

To reach the goal of the project, different set-up configurations, types of reactors and reaction parameters were tested. After a detailed screening, different compounds were synthesized in flow and good yields, up to 70%, were obtained in a very short residence time (40 seconds). Moreover, the scale up of the process was investigated [3].

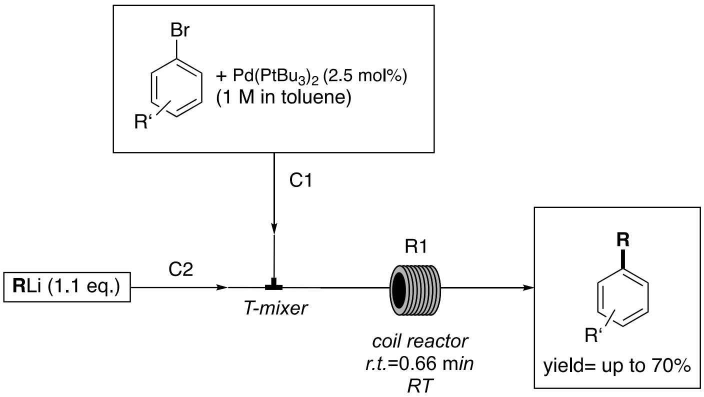

Figure 1: set-up and conditions for the general procedure.

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OR40

Enhancing Ecovio® Properties through Nanocrystalline Cellulose Incorporation

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The growing environmental awareness has spurred the research for sustainable alternatives to traditional materials. In this context, Ecovio® has emerged as a promising option due to its unique combination of mechanical strength, flexibility, biocompatibility, oxygen and moisture barrier properties that makes it suitable for various applications. It is a polymer composed of polylactic acid (PLA) and polybutylene adipate terephthalate (PBAT) derived from renewable resources, such as cornstarch and natural fibers, making it biodegradable and compostable [1]. As a biodegradable material, it offers a sustainable alternative to conventional plastics, reducing environmental pollution and waste accumulation but has some limitations: its mechanical properties are generally lower compared to traditional polymers. To overcome this, the use of additives, like cellulose nanocrystals (CNC), is essential [2]. CNC has a high specific surface area and remarkable thermal stability, also, its nanometric structure favors the interaction with the polymeric matrix, contributing to increase the mechanical and barrier properties of the composite. In this work we prepared composite materials of Ecovio® and CNC, modified by different approaches (acetylation, desulfation, TEMPO-oxidation and cationization), at 5 wt% and its thermal and transport properties were investigated, to observe how the use of these additives may modify the performance of the final materials.

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OR41

Innovative water-based electrolyte for DSSC as sustainable solvent

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In 2021 around 62% of the electricity over the world was produced by fossil fuels, and 28% was produced by renewable energy, in this case, less than 10% of electricity was related to wind power and solar energy [1]. The photovoltaics systems have been evolved over the years, from silicon photovoltaics systems, that is the most developed technology at an industrial scale, toward thin films devices and the so-called emerging technologies, such as Dye Sensitized Solar Cells (DSSCs), Organic PhotoVoltaics (OPVs) and Perovskite Solar Cells (PSCs).

DSSCs are of particular interest due to simple fabrication procedures, low-cost manufacturing processes and low dependence on the incident angle of irradiation. Moreover, DSSCs are highly wavelength-selective and could be designed as (semi)transparent, which allows DSSCs implementation in specific applications (agrivoltaic, indoor) where conventional technology could not be efficiently exploited. [2]

Nevertheless, the main drawback of DSSCs relies in the use, within the electrolyte formulation, of organic solvents (MPN, ACN, DMSO, EtOH) that are toxics, volatile and flammables [3]. Very recently, water-based electrolytes have been proposed as a valid alternative to organic counterparts. In this contribution, we resume our recent efforts in the development of aqueous and greener electrolyte: we developed different electrolytes (both in liquid and in semi-solid state) exploiting ready available materials and sustainable synthetic routes.

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OR42

Sustainable α-Fe_2O_3/g-C_3N_4 catalyst for high-pressure CO_2 photoreduction

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Nowadays the world economy is still based on the use of oil as an energy vector and the massive CO_2 emissions have become an enormous problem. When captured, CO_2 can be converted into more valuable product and photoreduction of CO_2 represent one of the most promising ways. One main problem is the very low conversion of the reaction, and Z-scheme heterojunction seems to be a possible solution to increase the catalyst efficiency. To make a Z-scheme possible, the two semiconductors should be stable against oxidation and reduction, such as hematite. This, together with the non-toxicity of iron oxides and the relatively small bandgap make it an excellent candidate for the exploitation of visible sunlight [1]. The fast recombination rate and the low energy of the conduction band, which represents the two main drawbacks of hematite, can be minimized exploiting a Z-scheme strategy [2] (Figure 1). Graphitic carbon nitride (g-C_3N_4) was directly synthetized by carrying out a sulphuric acid treatment [3] and α-Fe_2O_3/g-C_3N_4 have been later synthetized by in situ precipitation of $FeCl_3$ followed by a calcination at 350°C. Synthetized catalysts have been characterized though XRD, BET, DRS, SEM/TEM analysis and have been tested in a high-pressure setup under 18 bar of CO_2. The catalysts showed a productivity of formic acid between 5818 and 7335 mmol kg_{cat}^{-1} h^{-1}. It has been found that a very high loading of hematite causes a decreasing of the productivity of the catalysts. Furthermore, tests demostrated that the contact between the two semiconductors of a Z-scheme is a key parameter for the overall activity of a such type of catalyst.

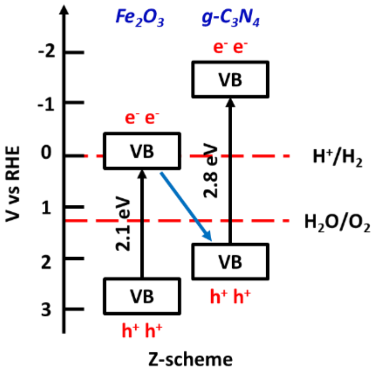

Figure 1: Schematic of a direct Z-scheme heterojunction.

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OR43

Aging-electric abuse of graphite/$LiFePO_4$ batteries from a chemical characterization perspective

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Lithium-ion batteries are currently leading the way towards the green transition in the transport sector. The graphite/$LiFePO_4$ (LFP) is the most widely used cell available on the market, due to its low toxicity, low cost and great cyclic performance. Although LFP-based batteries meet high safety standards, accidents are frequent and, even under guaranteed safety conditions, battery degradation occurs over time, during working and storage. To date, available research has been mainly focused on the study of the electrical abuse of batteries, carried out under severe conditions, in terms of overvoltage, to improve their safety [1]. On the other hand, also the study of aging under standard conditions is really attractive, to investigate the degradation under the normally used conditions and to find alternative applications of batteries when their original use is no longer permitted, leading to economic and environmental benefits. In this regard, in this work, experimental studies of aging were carried out on a commercial LFP cells with a nominal capacity of 40 Ah, thus representing realistic conditions of use for the automotive sector. More specifically, the cell has been subjected to a scaled current profile, corresponding to the stress to which the battery pack of an existing electric vehicle is subjected, when engaged in the conventional driving cycle today used for homologation tests (WLTP). In that way, the cell will be aged under realistic working conditions, thus allowing a fair comparison between the new and the used one. In this way, the pristine battery, considered as the benchmark, has been opened under an inert atmosphere, recovering cathode, anode and electrolyte. Information on the morphology of the cathode and anode is being obtaining by scanning electron microscopy, whilst the thermal characterization by differential scanning calorimetry will provide useful information on the deterioration on the battery performance upon aging completion [2]. The support of other characterization techniques, such as Fourier Transformed Infrared Spectroscopy, will complete the interpretation of the aging process.

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OR44

Monitoring the State of Health (SOH) of green batteries (GreenBat)

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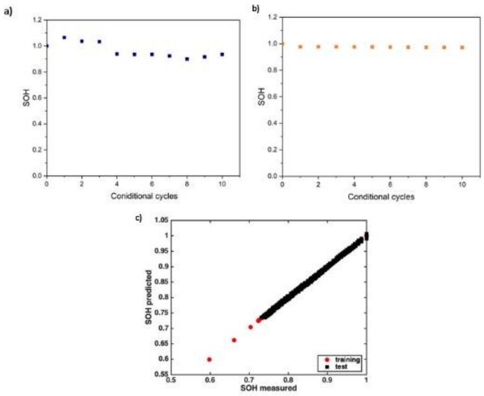
Here we focus on the study of state of health monitoring of secondary batteries with advanced “green” formulations. European recycle map on battery energy storage plans to replace positive electrodes consisting of cobalt (Co) and fluorinated (F) graphite-based negative electrodes constituents with environmentally sustainable alternatives. Recently, "green formulations" was validated; in particular, recent trends suggest the use of electrodes based on silicon (Si), Co-free manganites (LiMnO2) aqueous soluble binders and fluorine-free electrolytes [1]. Our aim is to describe the chemical and morphological changes occurring during the battery cycling, through spectroscopies (Raman and IR) operating in parallel with impedance analysis. These experimental data will be integrated with the electrochemical performance in a multiblock dataset, which will constitute the basis for chemometric processing. The purpose of this chemometric modelling is to correlate SOH evolution to the chemical and physical state of the battery [1]. Here we illustrate the analysis of SOH of two different pouch cells formulation constituted by LTO (Lithium-Titanate) as anode, LFP (Lithium-Iron-Phosphate) as cathode and the LP30 electrolyte (EC:DMC 1:1 and LiPF6 1M); the second formulation is constituted by a thin film layer of commercial Li metal (purity of 99.7%) as anode, LFP as cathode and an ethers based formulation as electrolyte. After formation cycles (CC-CV), the cells have been submitted to aging tests. The different operating conditions are chosen with an Experimental Design (ED). Turning to the chemometric modelling, as a starting point we verified the ability of PLS regression applied to the voltage profiles during charge cycles to estimate the SOH of a benchmark dataset by Lin et al. [1] (Figure 1c).



OR45

Structure and reactivity of bismuth vanadate-water interfaces

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Bismuth vanadate (BVO) is a promising photoanode for photoelectrochemical cells, due to its tunable band gap (~2.4 – 2.6 eV), favorable alignment of its valence band with the water oxidation potential, stability in aqueous environments, and its relative easiness of preparation [1]. In a recent study [2], we showed that tuning surface termination/composition and hence surface energetics is critical to improve the efficiency of the oxygen evolution reaction (OER) [2]. In addition, we highlighted [3] the importance of surface defects in altering the reactivity of BVO toward water, concomitant to water modifications to the electronic structure of the photoanode. However, a complete atomistic description of the interface between defective facets of BVO and water is not yet available, and yet it is necessary for the optimization of the OER efficiency. Here we carry out first principles molecular dynamics simulations with the Qbox code (http://qboxcode.org/) of BVO-water interfaces with different composition, as well as measurements of the electronic (XPS) and vibrational (IRRAS) spectra of water-covered BVO thin films. We combine theoretical and experimental results on spectra and computed electronic properties to characterize the interplay between surface hydroxylation and metal oxidation states at the surface, and to understand their impact on surface reactivity.

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OR46

Exploring nanoplastic pollution through realistic test materials: characterization, ageing and biological interactions

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Environmental plastic pollution is nowadays a main concern across all ecosystems.

Plastic wastes take hundreds of years to degrade, via abiotic and biotic degradation processes, leading to the accumulation of micro- and nanoplastics (MNPs) in all environmental compartments. Over the last decade, a significant amount of research has been conducted to assess MNPs distribution, fate and risks to organisms [1].

However, their limitation in size contributes to the lack of adequate methods for qualitative and quantitative studies. In addition, natural ageing mechanisms could alter phisico-chemical characteristics of MNPs and further hamper their sampling with available techniques. For these reasons, studies have been so far conducted using synthetic polystyrene nanobeads (NBs). There is a strong need to create good test materials for laboratory studies, mimicking as closely as possible the real MNPs [2-3].

In this contribution, a study of MNPs through the preparation of more realistic test materials, named here "true-to-life" MNPs, will be presented. True-to-life MNPs were produced from daily life plastic items subjected to mechanical fragmentation and ageing phenomena and characterized from both the chemical and the morphological points of view. The nanoscale behaviour of the interactions with biological system was investigated through the study of protein-corona formation from human plasma, by comparing raw and aged true-to-life NPs.

Figure 1: Closing the gap in micro/nanoplastics research: true-to-life MNPs as more environmentally relevant test materials.

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OR47

Biomonitoring strategies to assess metal pollution through analysis of lemurs biological, samples in Italy and Madagascar

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Metal-contaminated environments are common in urbanized areas due to their proximity to emission sources. Organisms can accumulate metals and other elements present in their habitat, mainly through ingestion and contact. In biomonitoring investigations, wild and domesticated mammals are frequently used. Animals housed in zoos, provide excellent opportunities to study the potential of a particular species as bioindicators: living in limited areas, they are more likely to reflect the environmental conditions of a specific zone. [1][2] The aim of this study is to test new non-invasive approaches for biomonitoring element content in the environment using captivity lemurs as target animals. The study was conducted partly in Italy and partly in Madagascar, to compare the data acquired from both sites. The study was possible thanks to the collaboration with Fondazione Zoom, an institution promoting research activities in Zoom, an Italian Biopark, and the collaboration with the Parc Botanique et Zoologique de Tsimbazaza, Antananarivo, Madagascar. The animal matrices chosen for the project were feces and fur. The results obtained with the analysis of those samples were compared with the mineral element content in other environmental compartments, namely water, and soil. In both parks, water, and soil were collected at different points of the lemurs' habitats while the zookeepers collected the animal matrices with appropriate protocols. Four species were included in the study: *Lemur catta, Eulemur mongoz, Eulemur rubriventer, and Eulemur macaco*. Thirty-four elements were taken into consideration. Multivariate analysis of the data made it possible to understand the relationships between the concentrations of the various elements in environmental compartments and animal matrices. The results highlighted the potential of using lemur feces and fur as bioindicators of element content in animal habitats. An added value of this work is the comparison between the data collected for the same species in their original area and the European one, focusing on endangered animals.

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OR48

Optimization of a flow-cell reactor operating parameters for the electrochemical ammonia production from wastewater

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Although its high carbon footprint, the Haber-Bosch (HB) process mainly dominates the NH_3 production market. The catalytic reaction between N_2 and H_2 requires high energy input, being carried out at high temperatures and pressures. HB plants are not evenly distributed in the world, thus NH_3 and its derivates transportation to the final user is a large portion of the overall environmental impact [1]. For these reasons, in the last years, the research has focused on the possibility of producing ammonia from direct nitrogen electrochemical reduction (NRR) in aqueous electrolytes under ambient conditions exploiting renewable energy. This process is limited by low selectivity at high current densities and low yield, due to the high dissociation energy of the N_2 triple bond and the unavoidable hydrogen evolution reaction (HER). On the other hand, NO_3^- can be easily converted into NH_3 thanks to the lower activation energy, which makes the reaction thermodynamically favoured compared to N_2 reduction [2]. Due to the massive agriculture, NO_3^- is one of the most abundant contaminants of underground waters. Thus, the use of NO_3^- to produce NH_3 under ambient conditions can be carried out with lower energy consumption, but can also address the water pollution issue [3].

The aim of our work is to assess the catalytic activity of commercial MoS_2 and a synthesised Bi-based catalyst in a gas-diffusion electrode flow cell of 10 cm^2 geometrical area. Design of experiments and surface response methodology (DoE/RSM) were employed to gain further insight into the influence of operational conditions (potential, catalyst loading and salt concentration) on the Faradaic efficiency and NH_3 yield. MoS_2 catalyst showed good catalytic activity towards NH_3, with a FE between 62%-77% and yields between 2.9-13 mmol g^{-1} h^{-1}. On the other hand, Bi material showed 21% FE and 0.41 mmol h^{-1} g^{-1}, probably due to Bi final oxidation state, which is not so active towards NH_3 production. NH_3 quantification has been carried out through UV-vis colorimetric method, using both Nessler's and Berthelot's reagents.

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OR49

Life cycle assessment of recipes served in food canteens and elaboration of a new environmental indicator

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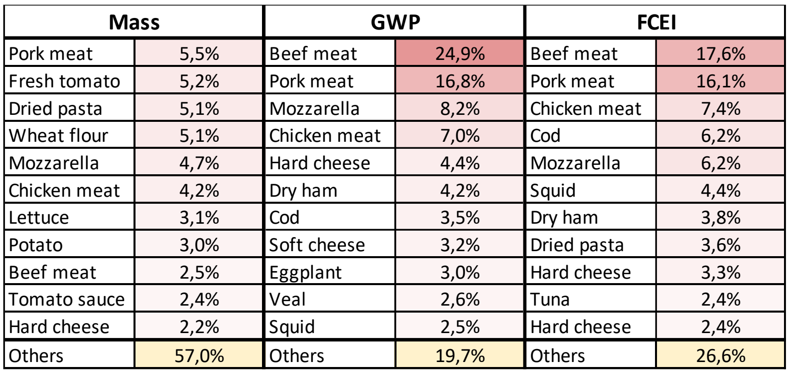
Many studies aimed at estimating the environmental impacts associated to the food sector, but most of the existing indicators limited the problem only to the climate change, while it is well-known that the issue may be extended on a wider spectrum of environmental categories[1]. In this work, the Life Cycle Assessment (LCA) was applied to a list of 1001 recipes (LoR) of an Italian food canteen, prepared with 150 ingredients, with the purpose to develop a comprehensive environmental indicator (namely, SQUIID, Simplified Quantitative Impact Indicator for food Dishes), including in the evaluation the categories showing a significant contribution (at least 86%) to the ReCiPe 2016 single score[2], i.e. global warming (GWP), particulate matter formation (PMFP), land occupation (LOP), human non-carcinogenic toxicity (HTPnc) and water consumption (WCP). The LoR was analyzed under three perspectives: mass, GWP and SQUIID impact. The mass perspective indicates that the LoR contains a fairly balanced amount of ingredients, pointing out a remarkable diversification of the menu in the canteen. Concerning GWP and SQUIID spheres, meat-based and fish-based recipes resulted the main impacting ones (77% for GWP and 73% for SQUIID), demonstrating to be the two classes mainly responsible for the impacts observed, even if the vegetarian and vegan courses represent the 41% in mass. Meat-based dishes represent the 42% of the entire LoR in case of GWP, when adopting SQUIID, their contribution is reduced to the 35%. In fact, the main percentage of SQUIID is attributed to fish, raising from 31% (GWP) to 43%. Such variation demonstrated the relevance of the four additional selected categories for a final evaluation, proving that GWP-based indicators provide to the consumer only a partial representation of the issue.



Mass		GWP		FCEI	
Pork meat	5,5%	Beef meat	24,9%	Beef meat	17,6%
Fresh tomato	5,2%	Pork meat	16,8%	Pork meat	16,1%
Dried pasta	5,1%	Mozzarella	8,2%	Chicken meat	7,4%
Wheat flour	5,1%	Chicken meat	7,0%	Cod	6,2%
Mozzarella	4,7%	Hard cheese	4,4%	Mozzarella	6,2%
Chicken meat	4,2%	Dry ham	4,2%	Squid	4,4%
Lettuce	3,1%	Cod	3,5%	Dry ham	3,8%
Potato	3,0%	Soft cheese	3,2%	Dried pasta	3,6%
Beef meat	2,5%	Eggplant	3,0%	Hard cheese	3,3%
Tomato sauce	2,4%	Veal	2,6%	Tuna	2,4%
Hard cheese	2,2%	Squid	2,5%	Hard cheese	2,4%
Others	57,0%	Others	19,7%	Others	26,6%

***Figure 1**: ingredient contribution on the total LoR per mass, GWP and SQUIID*

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OR50

Sustainable Ru-Supported Hydrochar from Biomass Waste for N-Containing Chemicals *via* Biomass Reductive Amination

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The conversion of biomass waste into catalysts and the production of valuable products through catalytic reactions represent a highly significant area of research, addressing both energy and environmental challenges [1]. This research aligns with sustainability goals, wherein hydrochar derived from the hydrothermal treatment of brewing industry waste was utilized as a support for a Ru-based catalyst (Ru-HC) in reductive amination. An efficient continuous flow protocol, coupled with a hydrogen source, achieves 99% conversion in hydrogenating LA and *n*-butylamine to pyrrolidones compounds. The Ru-HC's catalytic potential extends to diverse substrates encompassing various carbonyl-containing compounds and amines, including biomass-derived molecule platforms like furfural, 5-hydroxymethylfurfural, and furfurylamine, yielding valuable N-containing products [2]. Mechanistic insights are confirmed through intermediate formation and recyclability studies, highlighting Ru-HC's robustness and stability. Solvent selection and key parameters like flow rate, temperature, and pressure influence selectivity. The adoption of a continuous process reduces reaction times and eliminates the need for hazardous gaseous hydrogen, ensuring heightened selectivity. This research showcases an environmentally friendly method for producing high-value compounds from biomass, contributing to sustainable amine synthesis using biomass-based catalysts.

Figure 1: Schematization of waste conversion and its exploitation as a catalytic support

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OR51

Novel GC-MS human biomonitoring method for the quantification of legacy and emerging pollutants in serum samples

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Environmental research and public health in the 21st century look toward numerous challenges including the widespread use of substances that are potentially harmful to humans. Among the several anthropogenic pollutants present in the environment, persistent organic pollutants (POPs) are the most concerning compounds due to their adverse effects on human health and wildlife [1]. However, the restriction has led to the introduction of new chemicals now called "emerging contaminants" (ECs).

The urgent need to get a complete view of everyone's exposome meets the necessity to assess how and how much chemicals are actually absorbed from the environment into the organism itself, and whit the practical question of the methodology applied to measure the exposome itself. In this context, Human Biomonitoring (HBM) plays a crucial role in establishing exposure and risk assessment [2].

With the aim to contribute to the full characterization of the exposome, a new gas chromatography-mass spectrometry (GC-MS) method for the identification and analysis of a broad spectrum of legacy and emerging contaminants in serum samples was developed.

Design of Experiments (DoE) concept was used to optimize the MS assay, as well as critical method aspects such as chromatography separation, method sensitivity, and the extraction procedure of the target compounds in serum samples. From the chemometric evaluation of the data, a validated model was constructed, which allowed the estimate of conditions for optimum chromatographic analysis. The proposed method was validated to achieve high analytical performance in terms of selectivity, linearity (R2 >0.995), accuracy (bias%≤ 10%), precision (CV%≤ 10%), robustness, ruggedness, limit of detection, limit of quantitation, recovery, matrix effect, and repeatability according to the international guidelines.

The developed method represents a powerful tool that can be employed in HMB to investigate the impact of pollutants on human health, expanding the still limited knowledge about ECs.

This method will be useful in future applications on subjects at high risk of exposure to assess potential correlations between pollutant levels and disease development.

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OR52

Polyvinylpyrrolidone-capped Metal Nanoparticles: effects of size, metal and interaction with the capping agent on biomimetic cell membranes and *in vitro* cell model

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In this work, the physicochemical/biological properties of gold (Au), silver (Ag), and palladium (Pd) nanoparticles (NP), fabricated by green reduction of the respective metal salt precursors with glucose, in the presence the polyvinylpyrrolidone (PVP) stabilizing/capping agent, were investigated.

The physicochemical characterization of the PVP-capped NPs confirmed the PVP excellent properties as stabilizing agent (as indicated by DLS and optical spectroscopy analyses) and demonstrated different polymer-NP interaction mechanism, depending on the NPs size (evidence from ATR-FTIR and AFM).

Biophysical studies with model cell membranes of supported lipid bilayers (SLBs) made with 1-palmitoyl- 2-oleoyl-sn-glycerol-3-phosphocholine (POPC) dye-labeled with 7-nitro-2-1,3-benzoxadiazol-4-yl (NBD) and/or lissamine rhodamine B sulfonyl (Rh) showed the most significant perturbation of the membrane fluidity in the case of AuNP and PdNP, which caused a significant decrease in the FRET transfer efficiency.

The intrinsic properties of the NP as potential chemotherapeutics were also investigated by in vitro experiments on prostate cancer cell (PC-3 line), to analyze the effect of cell-NP interaction in terms of cytotoxicity, cell migration (wound scratch assay) and cytoskeleton actin perturbation. A dose-response effect in the terms of cytotoxicity and the inhibition of cell migration especially for PdNP was found. LSM analyses showed a preferential NP accumulation in the perinuclear region, and an increased stiffness in the actin filaments.

OR53

Hair cortisol as a biomarker of chronic stress, comparison between matrices

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Cortisol is a steroid hormone commonly known as the "stress hormone". Like all steroid hormones, it is produced from cholesterol. The steps leading to its synthesis take place at the level of the adrenal glands under the control of the hypothalamic-pituitary-adrenal axis. The main factors involved in controlling cortisol secretion are: negative feedback, stress-induced stimuli and circadian rhythm.

The rate of cortisol production shows high intra- and inter-individual variability and is related to a physiological circadian rhythm. Usually, cortisol levels were quantified in saliva, urine, or blood, to describe an extemporary, non-specific oxidative status [1].

Chronic hyper- or hyposecretion of cortisol is influenced by environmental factors, psycho-physical stress and involves long-term physiological changes.

Chronic stress can increase the susceptibility of the individual to developing diseases: in particular, several studies have shown that acute and chronic stress factors, can increase the probability to have heart events, such as heart attack.

Hence the interest in the use of cortisol as a biomarker for chronic stress, usable as a prognostic marker for many diseases but also as a predictor and therefore applied in the prevention field.

In literature, correlations between cardiovascular diseases and chronic cortisol levels, measured in biological fluids such as urine, blood or saliva, are described but there are not enough evidences that its amounts could be used as prognostic marker.

Cortisol levels in hair [2] determined by LC-MS/MS, in addition to other matrices, could be a reliable biomarker of long-term HPA axis activity since it reflects total cortisol production for several weeks or months and it is thought that the amount of hair cortisol is proportional to the concentration of systemic cortisol.

Since the hair has a growth rate that generally stands around 1 cm/month, the concentration of a compound in a specific hair segment is closely related to the exposure/production suffered by the subject in the period corresponding to the hair growth under examination. For this reason, cortisol levels could be quantified in hair analysis and could be correlated with chronic stress [3].

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OR54

“COUMARIN DERIVATIVES FOR NUCLEAR MEDICINE: TARGETING MCT1 WITH FLUORINE AND COPPER”

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MCT1 is a membrane protein responsible for the transport of lactate and other monocarbon units normally expressed in healthy tissues. However, in some cancer lines its over-expression results in aggressiveness and poor prognosis. This allows MCT1 to be a potential target for theranostic applications in oncological field [1]. To date, only few molecules acting as inhibitors for MCT1 are known [2], and their interactions within MCT1 pocket have been elucidated by Xray crystal data [3]. Coumarins are natural phyto-compounds that showed a large variety of biological activities. One of the recently developed MCT1 inhibitor (7ACC2) that reached clinical trials is a coumarin derivative, so this family of compounds deserves attention [2].

Starting with preliminary docking calculations, the structure of the 3-carboxy,7-hydroxycoumarin was modified to retain a high affinity for the protein structure and to insert an additional specific moiety that allows the radiolabelling with 18-Fluorine.

18-F usage is limited to diagnostic applications, our intention is to shift to the use of a bifunctional chelator (BFC) approach to envision Copper (II) isotopes radiolabelling. This would indeed permit to reach the so called “theranostic-pair approach” exploiting different copper isotopes (64-Cu and 67-Cu). A chelating system suitable for copper (II) must be grafted on the targeting vector while reducing the impact on the interaction with the target protein as much as possible. A specific design of the chelator must then be used including to preserve the overall charge of the radiopharmaceutical. For such goal, an “in-house” bifunctional polyazamacrocycle, namely ***no3py*** and its new analogue bearing sulfonic pendants (***no1py2pys***) to allow a neutral chelate will be conjugated on the targeting vector using a PEG chain as a spacer.

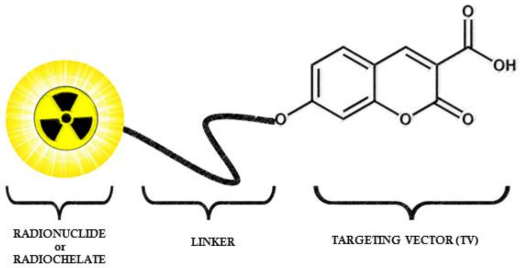

Figure 1: General structure of 3-carboxy,7-hydroxycoumarin derivative obtained.

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OR55

Site-selective functionalized PD-1 mutant endowed with immunological activity

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T-cells are essential for the immune system's adaptive response against pathogens and unhealthy cells, including cancer cells [**1**]. Key checkpoints that regulate the activity of T-cells' functions are Programmed cell death protein-1 (PD-1) and its ligands (PD-L1). Cancer cells overexpressing PD-L1 can inhibit T-cells leading to a tumoral microenvironment.

PD-L1 is currently a target for cancer immunotherapy and many monoclonal antibodies designed to bind the ectodomain of this transmembrane protein have been approved for clinical use.

In alternative, recombinant PD-1 ectodomain can hamper the PD-1/PD-L1 axis and can also be used as a vector to deliver therapeutic compounds, toxins, or probes to cancer cells that are overexpressing PD-L1 [**2**]. Particularly interesting is the possibility to employ recombinant PD-1 as carrier to address cancer cells with immune stimulating agents.

In this circumstance, L-rhamnose conjugated to peptides or proteins was successful in eliciting an immunological response by stimulating the production of anti-rhamnose antibodies, which in turn stimulated macrophages and lymphocytes [**3**].

Herein, we report on the design, biophysical characterization and site-selective rhamnosylation of a novel mutant of PD-1, presenting a nanomolar affinity towards PD-L1 and immunomodulatory properties.

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OR56

3D printed polycaprolactone/paper mill sludge prototypes: preparation and characterization

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Paper mill sludge (PS) is a high-volume waste of the pulp papermaking industry, containing calcium carbonate (70 wt%) and a minor amount of cellulose fiber (30 wt%). From a circular economy perspective, the exploitation of this material represents the only possible choice for a more sustainable future [1]. In collaboration with Lucart company, this research investigated the valorization of PS as filler in the preparation of polycaprolactone (PCL) composites. In fact, PCL is an excellent renewable plastic raw material with great mechanical properties and PS is a biomass waste with high potential due to the presence of cellulose and calcium carbonate [2].

PCL-PS composites were prepared with a PS loading in the range of 10-30 wt% by hot melt extrusion to obtain filaments. Then, a Fused Deposition Modeling (FDM) 3D printer was used for the fabrication of PCL-PS prototypes. FDM technology is a prevailing technique for numerous applications, from domestic to industrial ones, and it is employed for testing the feasibility of new process. A preliminary thermal and mechanical characterization of the new PCL-PS samples was performed, and the achieved results were compared with those obtained for neat PCL (Figure 1). In particular, the thermogravimetric analysis allowed us to investigate the thermal degradation profile, highlighting as the thermal stability of the composites slightly increases at the increase of filler loading. The mechanical properties, determined performing a three-point flexural test on 3D printed samples, show a more pronounced brittle behavior of the final material prepared with the highest PS loading (30 wt%).

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Figure 1: 3D printed samples of PCL and PCL-PS composites.

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OR57

Green technologies for chestnut wood extraction and fractionation

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In recent years a Circular Economy strategy and Green Extraction technologies [1] have been merged in common protocols. The efficient recovery of by-products from plant leftover, their fractionation and eventual conversion into new platform chemicals may generate relevant value. This approach represents a safe, cost-effective and sustainable strategy for the recovery of bioactives and their application in various fields such as nutraceuticals and cosmeceuticals. Chestnut wood (*Castanea sativa* Mill.) has been shown to be rich in several active molecules that exhibit diverse effects such as antimicrobial, antioxidant and anticancer properties. To explore the potential of sustainable and environmentally friendly protocols to recover enriched fractions of these metabolites, in this work Microwave-Assisted Subcritical Water Extraction (MASWE) have been employed on chestnut wood residues. By combining this methodology with green and easily scalable downstream technologies, two enriched extracts were successfully isolated. A two-step sequential extraction approach was used to pre-fractionate the product. To further increase the selectivity of polyphenols and tannins, the use of membrane filtration (ultrafiltration and nanofiltration, UF and NF) for downstream processing was then investigated. The UF retentate fraction had over 98% tannins, while the NF permeate contained up to 75.3% monomeric polyphenols [2]. Finally, the whole process was scaled-up to a pilot plant to demonstrate the suitability of this valorization approach for industrial purposes (up to 13 kg matrix and 150 L).

This case study highlights the untapped potential of a fractionation strategy that demonstrates the feasibility of sustainable recovery of bioactive compounds through the synergy of green extraction and downstream processing for new industrial applications.

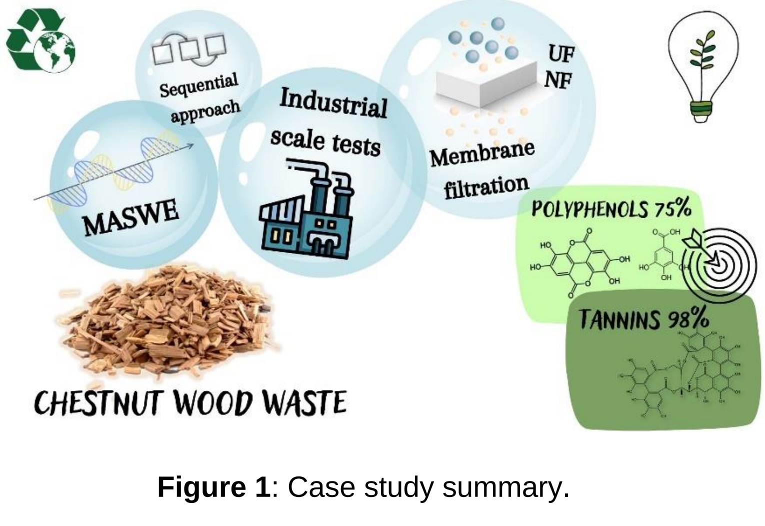

Figure 1: Case study summary.

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OR58

Synergistic effect of hydrodynamic cavitation (HC) and electrical discharge plasma (ED) for wastewater treatment: from target pharmaceutical compounds to a “hard-COD” real pharmaceutical industry effluent (PIE)

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Decontaminating pharmaceutical industry effluents (PIE) is of pivotal importance due to environmental and health risks associated with the presence of active pharmaceutical ingredients (APIs) and other contaminants. Extensive research efforts have been undertaken to remediate antibiotics, considering the lack of efficient methods for removing them from wastewater. Cavitation-based technologies are emerging as sustainable and greener alternative to wastewater treatment in the field advanced oxidation processes (AOPs) [1]. The production of hydroxyl radicals, hydrogen peroxide, ozone, UV light, and shock waves promoted by the synergistic effect of hydrodynamic cavitation (HC) and electrical discharge (ED) plasma has been studied for the intensification of tetracyclines (TCs) [2], metronidazole (MNZ) [3] and a real pharmaceutical industry effluent degradation process. Catalyst- and oxidant-free treatments have been carried out using a new pilot-scale hybrid device (HC/ED plasma) working in flow-through mode with different inlet pressure values (45 to 70 bar) on 5 L solutions and an average flow rate of 300 L/h. Near quantitative TCs (> 95%) and MNZ (90%) degradations were documented after only 15 min of combined HC/ED plasma treatment with the optimized operative conditions. A real PIE characterized by a starting chemical oxygen demand (COD) of 485 g/L was also treated inside the hybrid reactor, with a consequent highest COD reduction of 54% after only 10 minutes of treatment. To further increase the COD reduction, HC/ED treatments were performed in combination with oxidizing compounds (Oxone®, H_2O_2 and Fenton). However, no increase in the contaminants abatement was observed. Due to the recalcitrant behaviour of the treated PIE, the residual by-products of the optimized HC/ED treatment (i.e 54% of COD reduction) were removed from the water matrix using different concentrations (20, 40 and 60 mg/mL) of active carbon (AC), obtaining a complete water decontamination after 10 minutes of adsorption treatment with an AC concentration of 40 mg/L. Based on the results obtained, the combined HC/ED plasma process can be considered as a valuable, sustainable and industrially scalable alternative to conventional oxidation wastewater processes.

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OR59

Pure and high quality lignin from defatted and steam-exploded *Cynara cardunculus*

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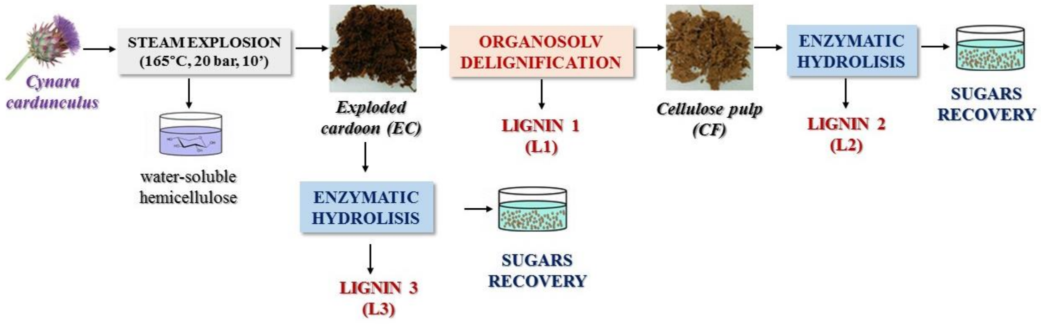
Cellulose, hemicellulose, and lignin are the three main components of the cell wall of a plant. The simultaneous valorization of cellulose and lignin is difficult to achieve because industrial processes entail methods that isolate carbohydrate polymers by lignin removal and degradation. Infact, biomass fractionation to isolate cellulose has been widely demonstrated, while isolation of useful forms of hemicellulose and lignin on an industrial scale is still under development [1]. Due to the prominence of aromatic derivatives in strategic chemical sectors, several areas have explored the use of pure lignin [2]. In this work, we describe a three-step approach to isolate the main components of lignocellulosic defatted *Cynara cardunculus*. After steam explosion, it was subjected to a mild *organosolv* treatment to extract soluble lignin (L1). Then, enzymatic hydrolysis was performed to achieve decomposition of the saccharidic portion into monosaccharides and isolate residual lignin (L2). This approach was compared with direct enzymatic depolymerization of cellulose and residual hemicellulose of defatted and steam-exploded cardoon (EC). In this way, we isolated valuable second-generation glucose and xylose and a final lignin-rich insoluble solid residue (L3). We performed several advanced characterization techniques on the three isolated lignins discovering the higher quality of L1 in terms of solubility and linear structure. Furthermore, the effect of the use of aqueous ammonia as a catalyst on the extraction outcomes was studied [3]. The Scheme 1 depicts the two fractionation approaches described above.



Scheme 1: Approaches to combined lignin and cellulose valorization of defatted C. cardunculus biomass.

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OR60

Eco-friendly and ready-to-market polyurethanes for LED encapsulation: substitution of toxic catalyst and fossil-based raw materials with a design of experiment approach

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In recent years, the use of polyurethanes (PUs) has witnessed a significant surge in industrial applications owing to their versatile synthesis routes and tunable physicochemical properties [1]. However, the widespread use of PU-based materials across various fields has raised notable environmental concerns, primarily associated with the extensive consumption of fossil-based raw materials and the utilization of mercury-based catalysts, which are now subject to stringent regulations imposed by European legislation [2]. Consequently, there is an urgent need to explore alternative reagents and catalysts with the aim of enhancing the sustainability of PUs by reducing resource consumption and minimizing the carbon footprint [3].

In this contribution, a commercial PU resin formulation for LED encapsulation has been investigated to implement bio-based and recycled components and remove the toxic catalyst while maintaining optimal characteristics in terms of optical transparency, physical and chemical properties. Specifically, a facile and solvent-free procedure will be presented for a new and eco-friendly PU formulation tailored for the optoelectronic sector. To achieve this goal, an Experimental Design (DoE) approach was successfully applied, and fossil-based components have been successfully substituted with bio-based and recycled alternatives in the optimized formulation. Bis(2-hydroxyethyl) terephthalate (BHET) was directly incorporated into the formulation as an example of waste-derived materials. Moreover, a combination of organobismuth and organozinc catalysts was effectively employed as a mercury alternative.

The optimized formulations not only retained market-level optical transparency but also maintained the desired physical and chemical characteristics throughout the optimization process, comparable to those of the commercial counterpart. This achievement paves the way for the development of a commercially viable, environmentally friendly PU formulation ready for market adoption.

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OR61

Nanocomposite based alginate and modified halloysite for potential use in food packaging

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In the last years, the design and development of nanocomposites which can be used in the food packaging field is rapidly increasing because of these occupy a central role in extending the shelf-life of foods preventing spoilage and possible adulteration. Different polymers have been successful used for this scope ranging from the plastic materials to biopolymers. The latter, being no toxic and often extracted from natural sources, are the most promising ones. Lately, the possibility to increase the physico-chemical properties of the polymers was investigated by adding fillers to the polymeric matrix. Among the different materials which can be used, inorganic nanoparticles have attracted considerable attention [1].

Halloysite nanotubes (HNTs) are natural clay minerals with a hollow tubular structure, consisting of a negatively charged outer surface composed of siloxane groups (Si-O-Si), and a positively charged lumen composed of aluminol groups (Al-OH). Due to the different chemical composition and the presence of an empty lumen, HNTs can be selectively modified onto the surfaces obtaining filler with improved interfacial properties with different biopolymers [2].

Herein, we report the synthesis of carbon dots (CDs) directly linked onto the external surface of halloysite using different both dicarboxylic acids and amines, as carbon source and passivant agent, respectively. The HNTs-CDs nanomaterials obtained were thoroughly characterized by a physico-chemical point of view and their morphology was investigated by transmission electron microscopy (TEM). Successively, the most promising HNT-CDs nanomaterial was used as filler to produce alginate-based nanocomposites, and the mechanical, physical and antioxidant properties of the obtained hydrogel were evaluated. Finally, with the final goal to employer the hydrogel for active food packaging, the HNTs-CDs nanomaterial was loaded with a natural extract know for its antimicrobial properties.

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OR62

Application of low molecular weight gelators to cosmetic emulsions

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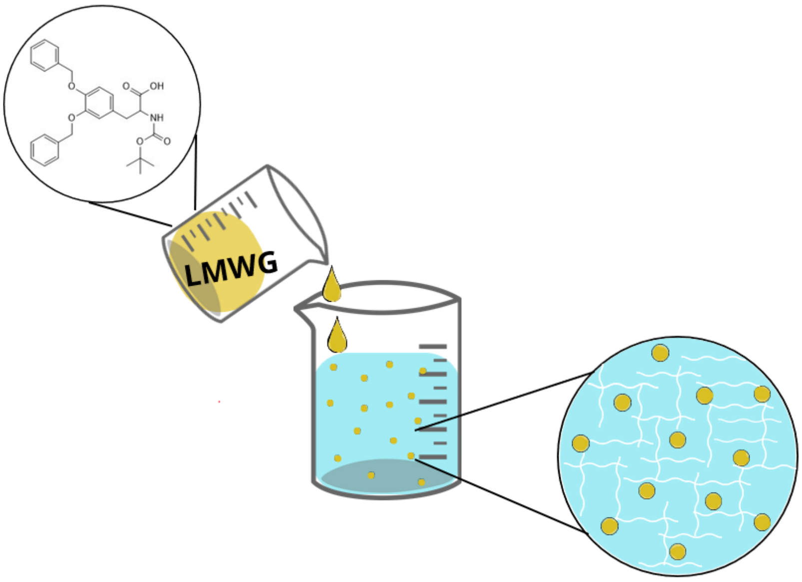
In the last few decades, polyacrylates have been widely used as raw materials in the cosmetic sector, since they provide an efficient control of the product viscosity. Unfortunately, these materials are poorly biodegradable in the environment, so the European Chemicals Agency (ECHA) is going to restrict their use in cosmetic products [1].

With the aim of replacing these polymers with more sustainable and biodegradable materials, we developed new formulations, using low molecular weight gelators (LMWG), that are small molecules that can self-assemble in fibers and form stable gels. Aromatic amino acids containing aromatic rings and polar functional groups are good candidates as LMWG, due to their ability to form weak bonds such as hydrogen bonds and π-π interactions [2].

In particular, we studied the application of Boc-L-DOPA(Bn)$_2$OH and Boc-L-DOPA(Bn)$_2$OMe to the formation of emulsions. We also analyzed the most convenient way to insert the LMWG inside the cosmetic formulation, discovering that their addition in the oil phase at high temperature leads to fast and complete dissolution. On addition of water phase, stable emulsions are formed, suggesting that these molecules could be suitable candidates to replace polyacrylates in cosmetic formulations.



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OR63

Ruthenium-based complexes as inhibitors of amyloid aggregation

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The aggregation of amyloidogenic peptides and proteins, leading to the formation of neurofibrillary plaques, is a characteristic feature of various neurodegenerative diseases including Alzheimer's disease (AD), Parkinson's disease (PD), Huntington's disease (HD), and dialysis-related amyloidosis (DRA). In the pursuit of novel therapeutics, numerous compounds have been investigated, and among them, transition metal complexes have emerged as potential lead compounds for the development of neuroprotective agents. Notably, Ru-based complexes have garnered significant attention due to their promising properties in overcoming cisplatin resistance in various cancer types, exhibiting low general toxicity and, more recently, in neurodegenerative diseases for their therapeutic potential in the context of neurodegenerative diseases [1]. Herein, we report on the ability of two different class of Ru-based complexes to modulate the amyloid aggregation of model amyloid systems, in detail, Ru(II)-based CO-releasing molecules featuring bidentate benzimidazole and terpyridine derivatives as ligands (CORMs) [2] and Ru-arene complexes bearing glucosylated ligands [3]. By means of different spectroscopic (e.g., fluorescence assays, UV-vis absorption, and electrospray ionization mass spectrometry) and microscopic (Transmission electron microscopy) techniques, their Mechanisms Of Action (MOAs) have been elucidated. Overall data highlight that Ru-based complexes modulate the amyloid aggregation and open new perspectives for their application in the field of novel neurodrugs

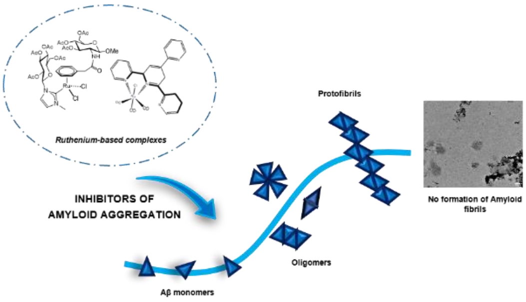

Figure 1: Schematic representation of Ru-based complexes mechanism of action.

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OR64

Engineering nanoceria for the protection of ancient frescoes

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Ancient frescoes undergo complex degradation phenomena that irreversibly alter the surfaces and compromise the structural integrity, putting at risk the historic and cultural legacy from the past. To avoid this loss, innovative conservative solutions are highly sought, and nanomaterials could answer this urgent need. Cerium oxide nanoparticles (CeO_2 NPs) have been gaining the interest of scientists due to their catalytic activity [1], and they can be the ideal candidates to fight difficult-to-tackle degradation phenomena.

A microwave-assisted synthetic protocol was developed to obtain high yield and high surface-to-volume ratio. Thanks to this optimized approach, highly uniform NPs with diameters below 3 nm were produced, as determined with advanced characterization techniques. Through UV-visible spectroscopy the oxidation of 3,3′,5,5′-tetramethylbenzidine (TMB) catalyzed by CeO_2 NPs has been monitored as a quick assessment of the catalytic performances. After this extensive characterization, CeO_2 NPs were included into a chitosan-based formulation [2], which was applied to mock-ups especially designed to replicate Roman frescoes. Preliminary tests of color alteration, hydrophobicity, and surface morphology were implemented, before and after artificial ageing, showing promising results in the development of advanced protective coatings based on CeO_2 NPs.

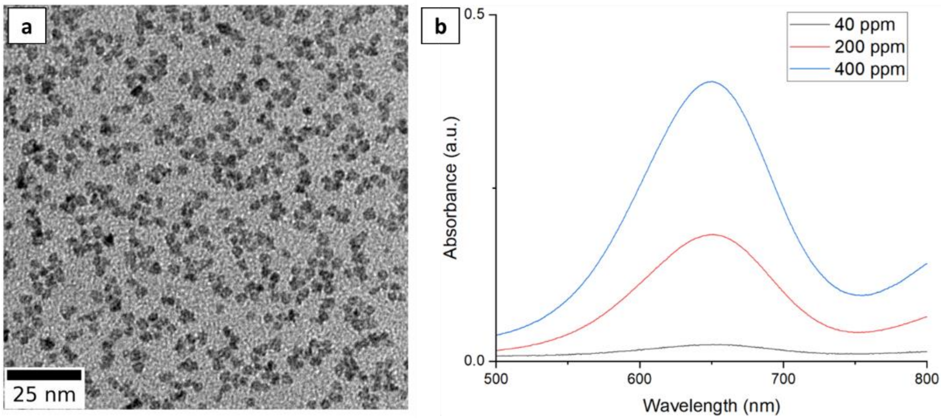

Figure 1: (a) TEM image of CeO_2 NPs; (b) UV-vis spectra of their redox activity.

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OR65

Liquid Crystalline Elastomers as starting point for contractile cardiac assist devices

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Heart Failure affects millions of people and represents a leading cause of death worldwide. This syndrome is associated with impairment of cardiac mechanical function. To assist ventricular contractility in patients affected by Heart Failure, left ventricular assist devices have been demonstrated able to reduce mortality in patients awaiting transplantation, but they are not suitable for long-term use. Moreover, current technologies can't restore muscular heart contractility.

The aim of our research is to develop a cardiac assist device based on a remote-controlled contractile tissue to assist or restore heart mechanical functionality.

The artificial muscle behaviors are exploited by the unique properties of Liquid Crystal Elastomers (LCEs). [1]

LCEs are smart materials consisting of rubber-like polymers made by chemically crosslinked liquid crystalline networks. These materials combine the entropic elasticity of elastomers with the orientational order at molecular level and sensitivity to different external stimuli of Liquid Crystals.

An increment of entropy, provided by an external stimulus (heat, light, electric field, chemicals), can perturb the order of the system, and this results in a macroscopic deformation of LCEs that can be exploited to generate movement or tension (Fig. 1) [1].

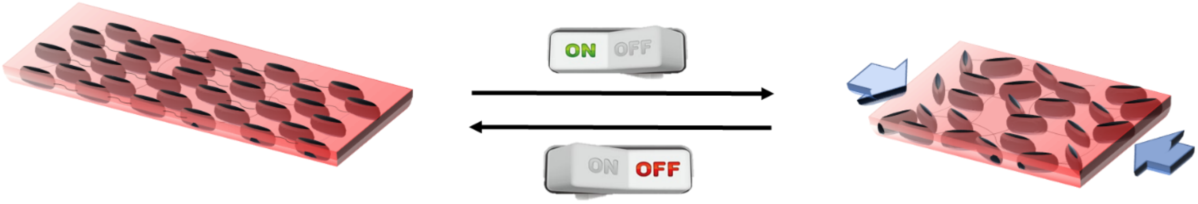

Figure 2: Scheme of LCEs actuation.

Different materials with different chemical compositions and architecture have different responsiveness (in terms of the amount of deformation, kinetics of activation and relaxation, and amount of tension generated) and different mechanical properties. Thanks to this, is possible to obtain a large palette of LCEs with tunable properties [2].

This work has received fundings for the European Union's Horizon 2020 research and innovation programme under grant agreement No. 95216 (REPAIR)

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OR66

Bifunctional iminophosphorane organocatalysts for enantioselective synthesis: application to the trifluoromethyl aryl ketimine nitro-Mannich reaction

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Bifunctional iminophosphoranes (BIMP) represent a class of so-named organic superbases which can be used as organocatalysts to promote several reactions. Thanks to their highly modular design, typically incorporating a variable H-bond donor moiety, a chiral amino acid-derived scaffold, and a phosphine-derived iminophosphorane superbase (**Figure 1A**), in recent years they have enabled unprecedented performances in enantioselective Brønsted base catalysis, allowing to access to high pK_a pronucleophiles [1].

Thiourea-based iminophosphorane organocatalysts featuring SPhos or BIDIME phosphine units, derived from the combination via Staudinger reaction of a chiral 1,2-amino alcohol-derived thiourea-organoazide with electron-rich phosphines, have been developed and successfully applied in the asymmetric addition of nitromethane to *N*-Boc-protected trifluoromethyl aryl ketimines (**Figure 1B**) [2]. *α*-Trifluoromethyl *β*-nitroamines, featuring a tetrasubstituted stereocenter, were obtained in good to excellent yields and enantioselectivities. The reaction was performed also on gram scale, without loss of enantioselectivity.

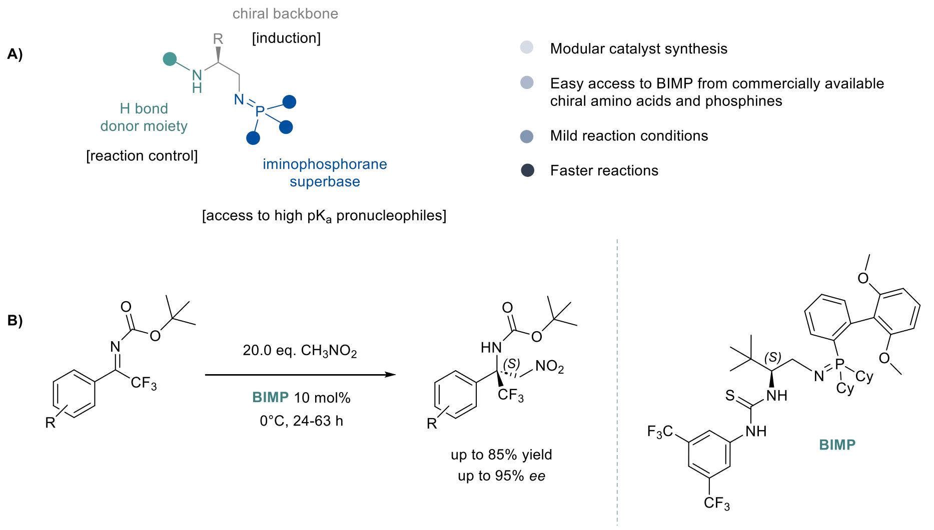

Figure 1: **A)** Key features of BIMP organocatalysts; **B)** BIMP-catalyzed synthesis of tetrasubstituted *α*-trifluoromethyl *N*-Boc protected *β*-nitroamines

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OR67

Hydroxyapatite: an eco-friendly support for enzyme immobilization

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High efficiency and selectivity, mild operational conditions and low toxicity are some of the main features that make enzymes efficient catalysts and important tools in making chemical processes greener. However, in order to render the process economically viable, enzymes should be recovered and reused and sometimes their operational stability needs to be improved [1]. A common strategy to tackle these problems is the immobilization of the enzyme on a solid support. Hydroxyapatite (HAP) is a biocompatible inorganic material which is suitable for this task thanks to its structural stability, non-toxicity, large surface area and ease of surface modification [2]. Moreover, it can be obtained from waste such as ashes from waste-to-energy plants, the fish supply chain, the avian supply chain, etc., in agreement with circular economy principles.

γ-glutamyl transferases from both *Bacillus subtilis* (BsGGT) and *Escherichia coli* (EcGGT) were chosen as model enzymes to study the immobilization process on HAP. HAP was synthesised according to a literature-reported procedure. Enzyme immobilization was initially attempted exploiting the electrostatic interactions between the charged groups on the surfaces of both HAP and the enzyme, simply by mixing an enzyme solution and a hydroxyapatite suspension under controlled conditions (pH, temperature). Different particle sizes and experimental set-up were investigated and the supported GGTs were tested as biocatalysts in the γ-glutamylation of L-methionine as a model reaction.

In the meantime, hydroxyapatite functionalization was studied to achieve covalent enzyme immobilization [3].

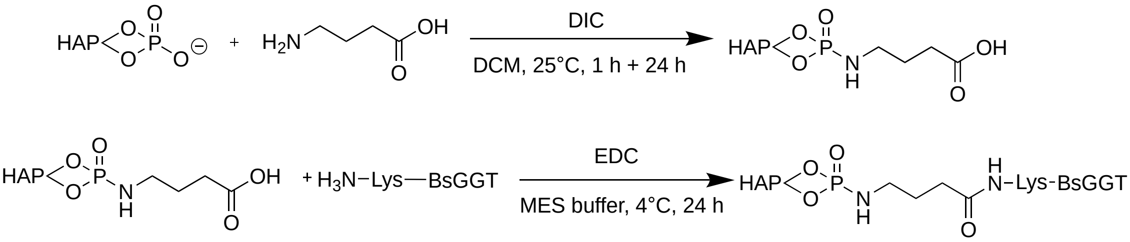

Figure 1: covalent BsGGT immobilization on hydroxyapatite

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OR68

In-situ and ex-situ thermocatalytic pyrolysis of plastics: a comparison of two different approaches

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Plastics are considered one of the greatest technological innovations of the past century and their production overcomes most man-made materials. Currently, only about 20% of plastic wastes are recycled, while 25% and 55% are respectively incinerated and discarded. In the last few decades pyrolysis became an interesting alternative to valorise plastic wastes by producing a wide range of products, from fuels to platform molecules, like olefins and BTX [1], [2]. The implementation of a catalytic stage allows a reduction in working temperatures and thus energy consumption compared to a purely thermal solution. Furthermore, the use of a catalyst could also improve the selectivity towards the condensable, most valuable, product fraction compared to the thermal solution. Acid catalysts (i.e. zeolites) can effectively reduce polymers' decomposition temperature and guide the reaction toward the desired products [3]. Two different approaches can be adopted to promote catalytic pyrolysis: in the "*in situ*" configuration the catalyst is loaded directly inside the pyrolizer together with the plastic mixture, while the "*ex situ*" mode has an additional, dedicated, heated reactor placed afterwards, which works on the partially cleaved molecules exiting the pyrolizer [3]. Despite being the simplest, the *in situ* approach has some drawbacks: i) the non-ideal contact between the fused polymer and the solid catalyst leads to mass and energy transfer limitations and ii) the recovery of the catalyst from the pyrolysis residue is challenging and, in some cases, not possible. On the other hand, the *ex situ* strategy, in which the catalyst is placed in a fixed-bed reactor, allows to improve mass transfer making trivial its physical separation after the reaction. Moreover, in the last case the conditions of both pyrolysis and catalytic upgrading can be independently optimized. Coke formation is a known cause of catalyst deactivation, but in the ex situ configuration, the catalyst can be readily regenerated. Some preliminary tests have been carried out in a "kettle type" reactor using zeolites with an *in situ* approach. They showed very promising results on the degradation of a mixture of polyolefins in different experimental conditions. All considered, the project aims to investigate multiple catalytic systems in a pyrolytic process to obtain the desired output. The final goal is to chemically recycle the "Plasmix" (plastic mix derived from waste sorting) to obtain useful products that can be reintroduced as feedstock in the chemical industry.

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OR69

Mechanistic study on the role of benzoquinone in the homogeneously catalyzed Guerbet reaction with a Ru-NHC complex

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Benzoquinone (BQ) was found as an effective co-catalyst in the Ru-NHC/NaOEt-catalyzed Guerbet reaction [1-2], which is widely investigated as a promising process for the conversion of bioethanol into more valuable chemicals such as n-butanol [3]. The co-catalyst behavior is here investigated through experimental and computational methods. The experimental results show an increase in both ethanol conversion (+25%) and higher alcohols yields (+18%), while the side-production of H_2 is reduced by 13%. DFT calculations were performed to investigate two hypotheses related to this kinetic effect: i) a hydrogen storage mechanism and ii) a basic co-catalysis of 4-hydroxiphenolate. The best theoretical results were obtained following the latter hypothesis, where a new mixed mechanism involving hydroquinone (the reduced form of BQ) as an alternative proton source to ethanol was found to be favored compared to the one catalyzed only by NaOEt.

A boost in process performance was experimentally recorded also with several phenol derivatives as co-catalysts, confirming that a stronger acid than ethanol could effectively improve the reaction kinetics of the Guerbet reaction.

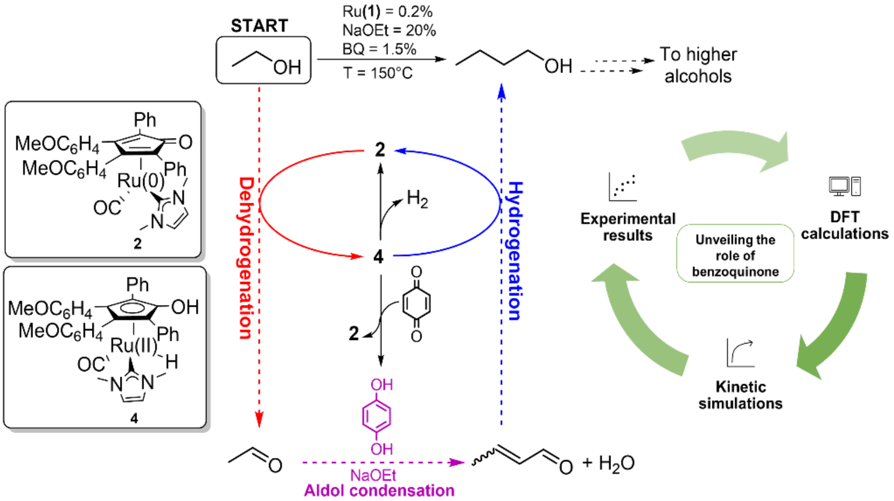

Figure 1. ***Mechanistic insight on the role of benzoquinone in the Ru-NHC/NaOEt catalytic cycle.***

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OR70

A bipyridine-based Cu complex as a candidate catalyst for C-H activation reactions: from the homogeneous to the heterogeneous phase

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The already known redox behaviour of a bipyridine-based copper (I) complex coded CuBPA[1], has been tested with a new selection of oxidant and reductant, revealing promising results in C-H activation reactions in the homogeneous phase[2]. Aiming at an industrial application, a catalyst working in the heterogeneous phase is usually more appealing, prompting us to develop the heterogeneous counterpart of CuBPA. The bipyridine backbone is particularly suitable as a linker in a Metal-Organic-Framework as long as it is decorated with carboxylic moieties necessary to ensure the possibility of connecting metal nodes in a UiO-67-like MOF. Hence, we first sought the best synthetic pathway to obtain the carboxylate bipyridine; different synthetic approaches have been tested for the less energy-consuming procedure with good yields and few steps. At this point, we successfully synthesized the desired UiO-67-type MOF by mixing the biphenyl-4,4′dicarboxylic acid linker with a controlled percentage of the synthesized bipyridine one, obtaining a stable MOF with enough active sites for Cu(I) grafting. Eventually, we finely tuned the condition for incorporating the copper metal centre: aiming at a Cu(I) site anchored to the bipyridine nitrogen atoms, we tested different (i) metal sources, (ii) impregnation solvents, (iii) ligand-to-copper ratios, (iv) MOF pre-treatments and (v) reaction environment. Finally, we are screening the best conditions to test the catalytic performances toward C-H activations of this new UiO-67-CuBPA MOF.

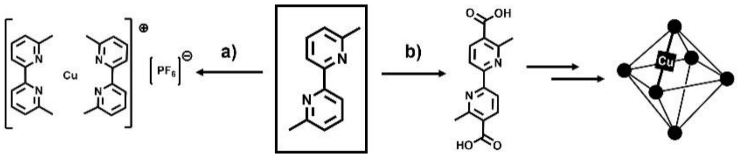

Figure 1: Routes toward the a) homogeneous catalyst and b) heterogeneous catalyst

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OR71

A multidisciplinary approach to detect stress symptoms in vegetable crops

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Crop losses due to stress factors significantly impact global food security, with abiotic stresses causing over 50% reduction in average yields of major crops [1]. The introduction of biotic stresses, like Fusarium wilt caused by *Fusarium oxysporum* f. sp. *lactucae*, severely affects lettuce growth, leading to significant losses [2]. Identifying strategies to prevent or mitigate these stresses has become a pressing concern. This study evaluates the effects of biotic and abiotic stresses on vegetables through a multidisciplinary approach, aiming to proactively detect stress symptoms and effectively manage them to maintain production quantity and quality. Lettuce (*Lactuca sativa* L. var. gentilina) was chosen as the model species, representative of widely consumed green leafy vegetables and suitable for hydroponic cultivation, known to enhance yield and product safety [3]. Two-week-old lettuce plants were transplanted into plastic pots with a peaty substrate mixed with perlite and cultivated in a closed, soilless system under controlled conditions. Stress treatments included water stress (W), nutrient stress (N), and biotic stress (B) induced by artificial inoculation with *Fusarium oxysporum* f. sp. *lactucae*. Biotic stress severity was assessed based on disease development and vascular browning (DS 0-100). Quality assessment and nutrient status analysis encompassed chlorophyll measurement *in vivo*, concentration of chlorophylls, carotenoids, phenols, anthocyanins, nitrate, sugars, and macro- and micronutrients (N, P, K, Ca, Mg, Cu, Zn, Fe, Mn, Se, and Mo) in dry matter. Proximal sensing technology, using a UV-visible-short-wave near-infrared spectroradiometer with a leaf clip tool, detected stress symptoms and predicted lettuce quality parameters. Spectral signatures of lettuce leaves were acquired at two time points during the growing cycle and processed using multiplicative scatter correction (MSC) and principal component analysis (PCA). A supervised machine learning clustering method was employed to classify the data into appropriate classes. Ongoing trials are expected to yield data from *in vivo* and destructive analyses, enabling correlation and optimization of the study and management of individual and combined stresses in leafy vegetables. The study employs a multiple response optimization approach, adhering to experimental design principles. Soilless cultivation systems offer precise control over climate parameters and inputs, resulting in efficient resource utilization. The proposed methodology shows promise for integration into a larger framework that combines different techniques and analyses to study stresses at various levels, improving their identification.

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[2] G. Gilardi, et al. *Plant Pathology*. Ed. 66 (2016) 677–688.
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Acknowledgements: This study was funded by the European Union Next-GenerationEU (PIANO NAZIONALE DI RIPRESA E RESILIENZA (PNRR) – MISSIONE 4 COMPONENTE 2, INVESTIMENTO 1.4 – D.D. 1032 17/06/2022, CN00000022) within the Agritech National Research Center. The views and opinions presented in this manuscript are those of the authors and do not necessarily reflect those of the European Union or the European Commission.

OR72

Stereostructural determination of a new cyanochelin from the cyanobacterium *Leptolyngbya*

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The marine environment hosts a huge number of micro- and macro-organisms, which are capable of producing and accumulating secondary metabolites and represent an incredible bioresource of biologically active and structurally unique natural products (NPs). The reasons for this complex multiplicity of secondary metabolites can be traced to a number of additional activities in which they are involved, such as intra- and inter-species communication, attack and defence mechanisms and adaptation to extreme environmental conditions, such as confined spaces, high ion concentrations and low food availability, which cause existing organisms to develop survival and defence mechanisms [1].

In this framework, our attention was paid to siderophores from cyanobacteria.

Cyanobacteria depend on great amounts of iron as an essential cofactor for metabolic processes such as photosynthesis, respiration or nitrogen fixation and have a greater need for iron than non-photosynthetic organisms. For this reason, they have developed many strategies to survive in limited iron conditions, such as the production of siderophores, which are compounds, secreted by microorganisms and plants, with low molecular weight (400-1000 kDa) considered the strongest chelators of Fe3+ [2].

Recent genome sequencing techniques and the detection of multiple silent gene clusters offer an excellent starting point for the identification of novel siderophores [3]. Using bioinformatic analysis and genome mining, additional gene clusters, presumably encoding for cyachelins biosynthesis, were identified. If iron-poor culture medium is used, it is possible to activate some silent gene clusters that may code for the production of unknown siderophores.

In collaboration with the research group of the Institute of Microbiology, in Třeboň, Czech Republic, a new cyanochelin from cyanobacterium Leptolyngbya sp. was identified and isolated. From the isolated cyanochelin sample, the stereostructural elucidation was studied through the combined use of mass spectrometry (MS) and nuclear magnetic resonance (NMR) techniques, mono- and bi-dimensional both homo- and heteronuclear, but also through the use of degradation and derivatization methods (such as the Marfey method).

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OR73

Acrylamide content and antioxidant activity among 8 different filter coffee extraction methods

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One of the undesired molecules generated during coffee roasting is acrylamide (AA)[1]. Despite the presence of AA, coffee is also a rich source of biologically active compounds with significant antioxidant properties, like polyphenols and chlorogenic acids. Therefore, the present work aimed to develop a comprehensive study and investigate the differences between the new filter coffee extraction method, Pure Brew (Victoria Arduino), with traditional ones (Turkish Ibrik, French Press, V60, Chemex, Clever, AeroPress and Moka), in terms of AA content and antioxidant activity. All analyses were carried out on three diverse coffees, belonging to *Specialty* and *Mainstream,* differently roasted (i.e., light, medium and dark). For the extraction of AA, purification of samples and its quantitation, a HPLC-MS/MS procedure was used[1]. On the other hand, analysis of chlorogenic and phenolic acids (antioxidants) and caffeine was performed according to a new HPLC-DAD method[2]. Antioxidant activity was determined spectrophotometrically by the DPPH method, while TPC and TFC of the different extracts were also performed. The results confirmed that the AA levels and antioxidant activity reached the maximum when coffee to water ratio used, for the same filter coffee extraction method, is higher, decreasing when this ratio for the same brew is lower.

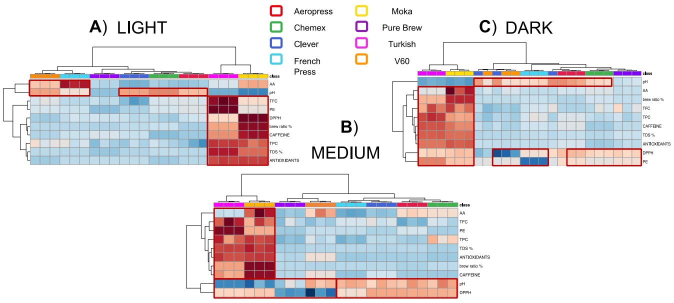

Figure 1: Hierarchical Heatmaps clustering comparing the different coffee extractions methods. Colors from red to blue indicate p-values from high to low; light cells indicate the lack of significant enrichment. **A)** Light roast **B)** Medium roast **C)** Dark roast.

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OR74

Chemiometric analysis for the traceability of high-quality Italian rice cultivars

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In recent years, the interest in rice (Oryza sativa L.) has increased, both from scientific research and the agri-food industry perspective. The need to preserve the authenticity of different rice varieties, especially those of high commercial value, has driven the research and development of advanced traceability technologies, such as Protected Geographical Indication (PGI) and Protected Designation of Origin (PDO) [1]. These certifications ensure the origin and quality of rice varieties, preserving their genetic diversity and contributing to the valorization of local productions. Italy, recognized as the primary rice producer in Europe, boasts a remarkable variety of cultivars and biodiversity. Within this context, the study aims to preserve the authenticity and integrity of valuable Italian rice varieties, by promoting the development of specific traceability technologies for Italian cultivars with PGI and PDO designations. To achieve this, several PDO varieties from the Baraggia region, including Carnaroli, S. Andrea, and Arborio, were directly collected from various producers. Additionally, the Carnaroli variety was sampled in different Italian production areas, such as Piana di Sibari (CS), Valle Lomellina (PV), Roseto degli Abruzzi (TE), and the Carnaroli PGI rice "Delta del Po." All these samples were meticulously characterized using various analytical techniques, including Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy (ATR-FT-IR), Multivariate Image Analysis (MIA), and Inductively Coupled Plasma-Mass Spectrometry (ICP-MS). The first two techniques allowed the development of rapid, efficient, and environmentally friendly methods suitable for rice quality control, while the latter, despite its high cost and the need for proper sample pretreatment, provided valuable information on the mineral fingerprint of the cultivars and their geographical origin. Finally, the instrumental analysis data were processed, yielding excellent results, using chemometric approaches to obtain information on traceability, geographical discrimination, and authentication of the analyzed Carnaroli PGI and PDO rice cultivars.

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OR75

Bio-orthogonal non-canonical amino-acid tagging (BONCAT) of pancreatic ductal adenocarcinoma

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Pancreatic ductal adenocarcinoma (PDAC) has a very poor prognosis, with less than 10% of patients alive five years after diagnosis. The prognosis of cancer patients is much improved through earlier detection. A recent study reported 5- and 10-year survival rates of 49% and 31%, respectively, for T1-2, N0, and R0 tumors[1]. Earlier diagnosis would enable treatment to begin when the tumor is in its earlier stages, and so improve patient prognosis. This aim would be achieved by developing a method able to isolate and identify characteristic markers of PDAC.

PDAC is characterized by a robust fibroinflammatory response, widespread vascular collapse, and hypoperfusion that make the tumor highly hypoxic and nutrient deprived. This microenvironment promotes tumor invasion, and progression leads to chemotherapy or radiotherapy resistance and eventual mortality.

To isolate newly synthesized protein from hypoxic cells we developed and optimize a protein labeling approach that is cell-type/phenotype-specific, and enables the solation through the labeled proteins. Bio-orthogonal non-canonical amino-acid tagging (BONCAT) is a technique that labels proteins with an azido moiety.

The azido moiety is introduced during protein synthesis using methionine surrogates, then with a simple click chemistry reaction, only the proteins that contain the azido moiety will be enriched[2].

Cell-specific BONCAT labeling can be achieved using azidonorleucine (ANL) as the Met surrogate. ANL is only incorporated into proteins by a specific mutant form of the protein methionyl-tRNA synthetase (MetRS*). Accordingly, ANL labeling can be restricted to cells equipped with this mutant form. The DNA of MetRS* is introduced into cells by transduction, using specific promoters to target specific cell phenotypes (e.g. HIF1α for hypoxia). Once ANL has been added to the media all methionines in the newly synthesized proteins from MetRS* transfected cells will be substituted for ANL.

Here we will show progress in method development, including results showing the incorporation of BONCAT labels into PDAC tumor cells and their enrichment by optimization of the click chemistry reaction.

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Flash presentations

FL01 – Di Pede Andrea Celeste (UniROMA2)
FL02 – Vit Margherita (UniUD)
FL03 – Franzini Marcello (UniTO)
FL04 – Maruzzo Valentina (UPPA)
FL05 – Priola Emanuele (UniTO)
FL06 – Urciuoli Gaia (UniPG)
FL07 – Berti Marco (UniBO)
FL08 – Forti Francesca (UniBO)
FL09 – Giorgio Anna (UniPD)
FL10 – Giuffrida Stefano (UniPA)
FL11 – Leveraro Silvia (UniFE)
FL12 – Nespoli Luca (UniMI)
FL13 –Lembo Antonio (UniNA)
FL14 – Culletta Giulia (UniPA)
FL15 – Milanesi Francesco (UniFI)
FL16 – Cataldini Simone (UniSI)
FL17 – Villaccio Rosa (UniNA)
FL18 – Armano Edoardo (UniMI)
FL19 – Daoud Razan (UniSI)
FL20 – Bonaldi Lorenzo (UniPI)
FL21 – Gallo Davide (UniTO)
FL22 – Verdoliva Valentina (UniCAMPANIA)
FL23 – Pace Alessandra (UniSI)
FL24 – Salvi Matteo (UniSI)

FL25 – Landi Alessandro (UniSA)

FL26 – Ranieri Simone (UNIVPM)

FL27 – Rossi Eleonora (UniBO)

FL28 – Mangini Anna (PoliTO)

FL29 – De Caro Silvia (IUSSPAVIA)

FL30 – Marconi Alessia (UniBO)

FL31 – Flammini Soraia (IRCCS AOU Policlinico San Martino-IST)

FL32 – Mannella Iole (UniTO)

FL33 – Masetti Andrea (UniBO)

FL34 – Ciarleglio Gianluca (UniROMA1)

FL35 – Fuochi Neri (UniFI)

FL36 – Morano Camillo (UniMI)

FL37 – Toldo Sofia (UniFE)

FL38 – Trotta Caterina (UniPG)

FL39 – Visentin Luca (UniBO)

FL40 – Marconi Riccardo (UniCAM)

FL41 – Lamonaca Antonella (ISPA-CNR)

FL42 – Iapadre Debora (UniVAQ)

FL01

Improving the specificity of CRISPR-based sensing platforms using Triplex-DNA

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The extensive use of CRISPR technology for diagnostic applications has been driven by the discovery of the collateral a-specific cleavage activities of CRISPR type V (Cas12) and type VI (Cas13) systems induced by DNA/RNA binding. In particular, Cas12 is an RNA-guided enzyme that integrate single- and double-stranded DNA target recognition, with signal amplification in one system [1]. The collateral cleavage is activated upon binding and is responsible for signal generation, for example, by taking advantage of the Cas12-mediated digestion of single-stranded DNA probes functionalized with a fluorophore-quencher used as fluorescence reporters [2].

Here, we describe a strategy for controlling Cas12a cleavage activity by using a rationally designed DNA-based hybridization network based on the formation of Clamp Triplex DNA. Clamp Triplex are DNA probes that can recognize homopurine DNA/RNA target with superior specificity and affinity compared to standard linear or hairpin DNA probe. When a ssDNA target is present, the Clamp Triplex probe alters its conformation that is associated to a reaction network leading to Cas12a activation and fluorescence output. Our molecular design allows us to overcome two hurdles that limit the application of CRISPR-Cas systems in diagnostics: we are able to distinguish with high specificity a single mutation base on the target sequence comprised between 10 and 20 nt by maintain the same LOD of standard CRISPR-Cas12-based detection systems.

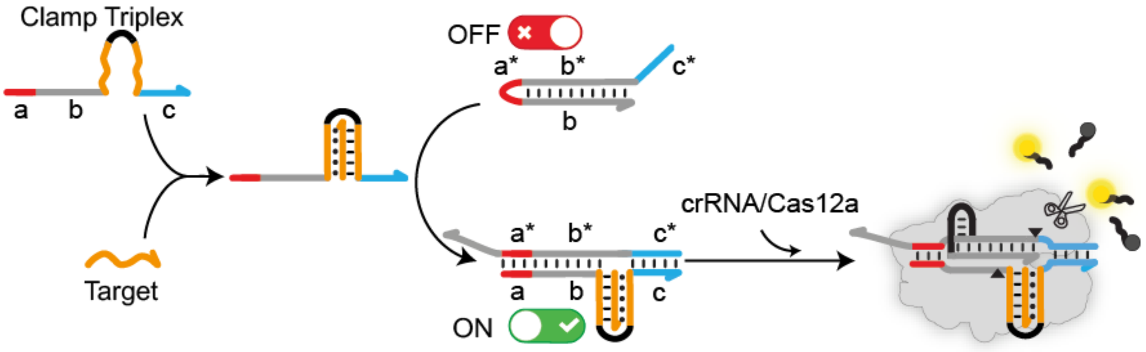

Figure 1: Schematic for controlling Cas12a trans-cleavage activity based on DNA-based hybridization network.

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FL02

Screen-printed E-aptasensor for Okadaic Acid (OA) detection

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Okadaic Acid (OA) is part of a toxin’s family produced by phytoplankton. These toxins can concentrate in filter-feeding shellfish and cause diarrheic shellfish poisoning (DSP) syndrome in consumers ingesting them. In European Union the maximum permissible level of OA (Regulation (EC) N.853/2004) is 160 µg kg^{-1}(*i.e.* 180 nM) and during the algal bloom period often the harvesting of shellfish is precautionally stopped with negative economical impacts. Instrumental detection is performed by chromatographic approach and devices for early detection and quick tests are so of interest. Recently aptamers (*i.e.* short sequences of DNA or RNA) are gaining popularity thanks to their cost-effectiveness, stability and customized synthesis [1]. Here is presented the optimisation of an electrodeposited gold-modified screen printed aptasensor for OA detection, based on“OA63”aptamer((Fc)5’CCGGGTGGGTGGGTGTGGTCTTGTATTTGATTATGTCTGTCGGCGCTTTTTGGCC**CCTTCGTT**-3’). Two purposely designed thiol-modified capture probes ie, P63-8((SH)5’-**AACGAAGG**-3’), P63-16((SH)5’-TTTTTTTT**AAGCAAGG**-3’) are tested. The “aptamer-capture probe”(A-C) hybridation in homogeneous phase (Fig.1A) and the preparation of the gold screen printed electrodes (Au-SCPE) were performed with protocols previously optimized by us. DTT (1,4-dithiothreitol) is used to activate SH-moiety of the capture probe through which the aptamer is immobilized overnight at 45°C @ Au-SCPE. The E-aptasensor OA63- P63_8 performed better in detecting OA in the range 5-200 nM with a DL of 2.5 nM (Fig.1B), which is well below the level imposed by law. We argued that the key step is the capture probe and the consequent 3D organization of the A-C complex in solution. The extra 8 thymines of P63_16 give too much degree of freedom to the aptamer apparently decreasing binding affinity to OA in the detection step. Instead P63_8 has 8 complementary bases to OA63 that give adequate stability to the structure that favors interaction with OA.

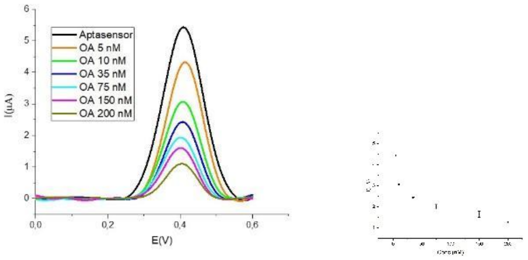

Figure 1: Preparation scheme of E-aptasensor and okadaic acid (OA) detection

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FL03

Doping strategies of thermoelectric organic polymers to enable efficient energy harvesting at low temperatures

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About 70% of the total energy consumed is wasted as heat, especially at low temperatures (<200 °C) [1]. It is therefore evident that collecting part of dissipated heat, and transforming it into electrical energy, is a crucial aspect to achieve for a more sustainable society. In this context, organic thermoelectric materials (OTEs) acquired significant interest toward the heat-to-electricity transformation because of several advantages, such as, mechanical flexibility, low material cost, light weight, low toxicity and increased sustainability [2]. In particular, polythiophene-based polymers, have attracted considerable attention due to their solution processability, chemical and thermal stability and high field-effect mobility. Generally, to exhibit proper thermoelectric behaviour a material should have low thermal conductivity, high electrical conductivity and high Seebeck coefficient. Nevertheless, the increase of electrical conductivity is usually coupled with an increase of thermal conductivity and a decrease of Seebeck coefficient thus limiting the overall efficiency, at least in conventional inorganic materials [3]. P3HT and PEDOT:PSS have been synthesized and optically, vibrationally, and thermally characterized. The effect of doping on electrical resistance and thus on optical and vibrational properties has been investigated. The electronic states tunability has been evidenced by doping the P3HT with anhydrous iron trichloride ($FeCl_3$) in acetonitrile at different molar concentrations and by detecting the formation of polarons via VIS-NIR and IR spectroscopy. Different dopants such as $FeCl_3$, I_2 and LiTFSI have been investigated and the stability in air and N_2 was examined. Several post treating methods have also been developed to boost the electrical conductivity and thus the TE performances of PEDOT:PSS, such as H_2SO_4, NaOH, MeOH, $LiClO_4$ treatments. Afterwards, these materials will be thermoelectrically characterized to figure out the optimum doping level to get an efficient TE material. In conclusion, polythiophene-based polymers are promising candidates to recover energy at low temperatures in different systems such as sensor networks, mobile devices, vehicles and buildings.

Acknowledgements: A.R. acknowledges the partial financial support from the Department of Electronic Engineering of the University of Rome Tor Vergata under the project "AIDED - Progetto di Ricerca Dipartimentale". M.F. acknowledges the support of Martur Italy srl.

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FL04

Synthesis of stable Hole Transporting Materials for Perovskite Solar Cells

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Perovskite Solar Cells (PSCs) are normally made up of a perovskite active layer, responsible for the charges generation, sandwiched between a layer of Electron Transporting Material (ETM) and a layer of Hole Transporting Material (HTM), to efficiently drain the charges towards the corresponding electrodes. In few years of research, impressive performances above 20% have been reached [1]. However, the limits in the long-term stability of PSCs still hampers their commercialization. The necessity to dope the HTMs constitute one source of instability, as the used agents are highly hygroscopic and favor the Perovskite degradation. Hence, HTMs are now being developed to get high efficiency in the absence or low concentration of dopants [2,3].

In this context, the present research aims at synthesizing and characterizing small molecules and polymers HTMs starting from phenothiazine and carbazole, low-cost and energetically tunable scaffolds. The study of the performances once implemented in the direct and inverted devices is ongoing.

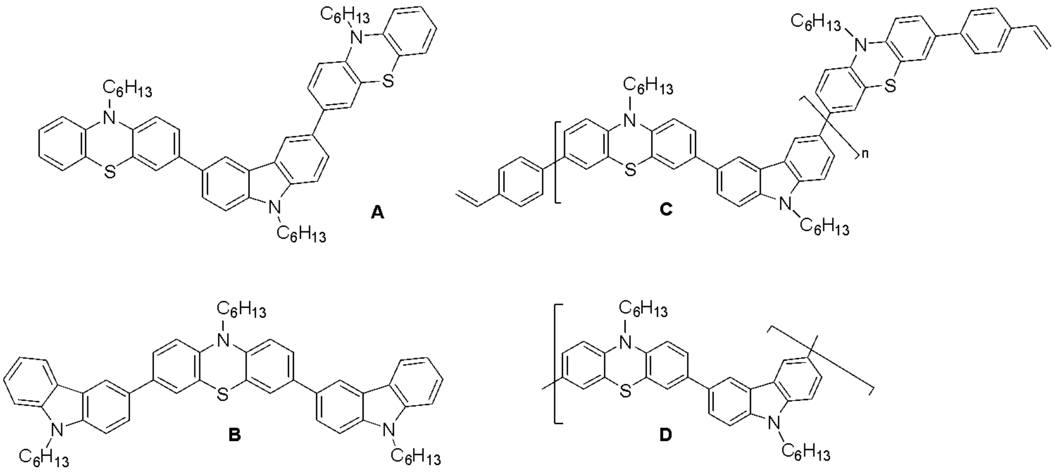

Figure 1: Small molecules and polymers HTMs.

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FL05

Gold(I/III) Perovskites for photovoltaic applications: from molecular structure to intermolecular interactions

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In the last decade, an enormous amount of work has been focalized on the analysis, synthesis and optimization of new perovskite materials for their very promising photovoltaic properties. The main mazterials are based on lead(II) halides, but with problems of stability in the real atmosphere and possible toxicity [1]. For these reasons, many combinations of +1/+3 metal centers have been analysed with very different performances. Recently, a new focus on mixed oxidation state gold halide perovskites reappeared [2]. Although the purely inorganic examples are known from a lot of time, very few organic-inorganic perovskites have been reported, and their use in photovoltaic show very interesting results. However, no one perform an in dept study on the forces of this solid, both at a molecular level or at a supramolecular level. In this work, we present a clean synthesis of four polymorphic ammonium and alchilammonium perovskites, their crystal structure and stability. At the same time, we performed calculation to demonstate the distribution of the charges into the gold(III) unit, in the framework of the inverted ligand field theory, and with QTAIM, NCI plots and ELF analysis, we manage to characterize the halogen/coinage Au⋯I contacts, that are at the basis of this family of solids [3]. We are sure that the results will shed new light on this fascinating and promising materials.

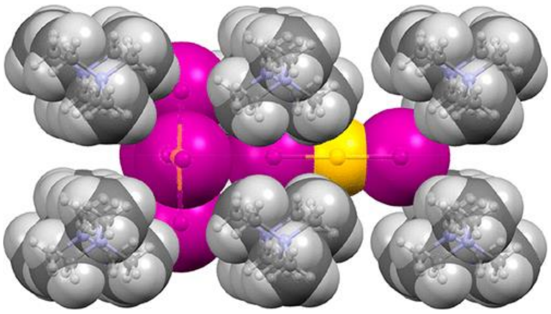

Figure 1: anion-anion interaction in tetrametylammonium derivative.

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FL06

Well-defined and “complete” Al-cocatalysts for olefin polymerization

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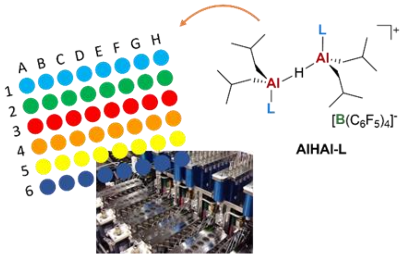
The performances of molecular catalysts for olefin polymerization are crucially dependent on the choice of the activator. Despite their fundamental role in precatalyst activation, cocatalysts have seen only limited advancements in the last decades [1].

Recently, we reported the discovery of a new Al-based cocatalyst, that is an unusual homodinuclear cationic species with two Al centers bridged by an hydride ($\{[iBu_2(PhMe_2N)Al]_2(\mu\text{-}H)\}^+[B(C_6F_5)_4]^-$, AlHAl, Figure 1) [2].

This species combines the ability of acting as abstractor, alkylator, and scavenger like methylalumoxane (MAO) with a defined molecular structure typical of borate salt activators. The efficacy of the AlHAl as cocatalyst relies on the coordinately saturated Al-centers possessing “latent” Lewis acidity. This new co-catalyst is easily synthesizable, stable at room temperature, and amenable to structural variations; it can therefore be considered the prototype of a new class of activators [3]. In this respect, we are synthesizing and testing a variety of AlHAl analogues differing for the nature of the donor (L), aiming to tune the latent Lewis acidity and gain insights on the factors determining cocatalytic properties. The synthesis of AlHAl-L analogues will be discussed, also highlighting the unexpected side-reactivity observed in some cases, along with the performances of this new class of activators in olefin polymerization with various catalysts. In particular, results of a systematic screening in a parallel pressure reactor (PPR) high-throughput experiment (HTE) platform will be presented.



DPI
Shaping polymer
innovation

Figure 1: Schematic representation of a high-throughput screening at varying donor L.

This research forms part of the DPI research program, project #857

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FL07

Sustainable synthesis of dimethyl adipate from cyclopentanone and dimethyl carbonate

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Dimethyl adipate (DMA) and adipic acid find wide industrial application in the production of nylon 6,6 (>10 Mton/y), a polyamide extensively used by the textile industry. Nowadays, adipic acid is mainly produced via nitric acid oxidation of KA oil, which is a mixture of cyclohexanone and cyclohexanol obtained from the oxidation of fossil-based benzene. The environmental impact of this process is extremely high, due to the emissions of NO_x and N_2O [1]. Indeed, it was decided to investigate and develop an alternative synthetic strategy for the production of DMA using cyclopentanone (CPO) and dimethyl carbonate (DMC) as reagents and working under liquid phase batch conditions, in presence of a heterogeneous catalyst to promote the reaction. Catalytic tests were conducted in compliance with the principles of Green Chemistry. In fact, both reagents can be obtained from renewables: CPO can be obtained from the processing of hemicellulose [2] and DMC from the condensation of methanol and CO_2 [3]. Furthermore, DMC acted both as solvent and reagent and the desired reaction pathway has a 100% atom efficiency. Different metal oxides and mixed metal oxides were tested, to assess their ability to promote the desired reaction pathway. Interestingly, a DMA yield of 40% was obtained after 5h of reaction, working at 260°C and in presence of a Zn/Mg mixed oxide. Deepening the mechanism investigation, it was found that the second step is limited by the low availability of the co-formed methanol for the nucleophilic attack over the beta-ketoester intermediate (carboxymethylcyclopentan-2-one). Indeed, this consecutive reaction step (Fig. 1), was investigated separately and a 92% yield of DMA was obtained in the optimized conditions (MeOH : Int = 150 : 1, cat: Zn/Mg/O 20%wt, T = 160 °C, t = 3 h, P = 20 bar). Subsequently, the assisted tandem catalysis strategy has been investigated. Using the same catalyst, the reaction has been performed in two steps, adding methanol between the two and obtaining a further improve in DMA yield.

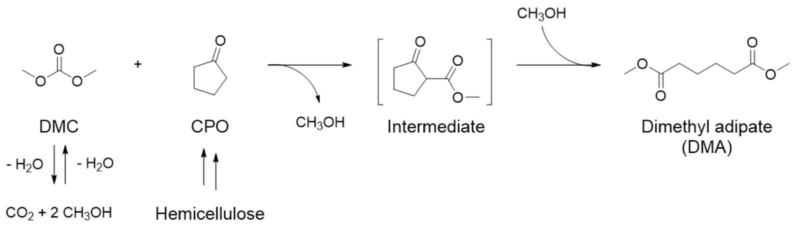

Figure 1: Reaction scheme for the production of DMA.

[1] M. T. Musser, *Adipic Acid, ULLMANN’S Encyclopedia of Industrial Chemistry*, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim 1 (2015) 537-548
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FL08

Synthesis and characterization of chiral $[(\mu\text{-H})_3Os_3Rh(CO)_{10}(\text{diphosphine})]$ clusters and study of their catalytic activity in asymmetric hydrogenation

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Four new osmium-rhodium tetranuclear chiral clusters of the general formula $[(\mu\text{-H})_3Os_3Rh(CO)_{10}(1,1\text{-P-P*})]$ (P-P* = chiral diphosphine of the ferrocene-based Walphos family) have been synthesized and characterized. The phosphorus atoms of the diphosphine ligands were found to be coordinated in a chelating mode to the rhodium atom [1]. The clusters have been tested as catalysts for asymmetric hydrogenation of tiglic acid [trans-2-methyl-2- butenoic acid] (Figure 1 b) [2].

The catalytic reactions gave conversion rates of 45-57% and enantiomeric excesses of 11-39% under mild catalytic reaction conditions. The crystal structures of $[(\mu\text{-H})_3Os_3Rh(CO)_{10}(1,1\text{-W002})]$ **2** and [(μ-H)3Os3Rh(CO)10(1,1-W009)] **4** are presented (Figure 1 a).

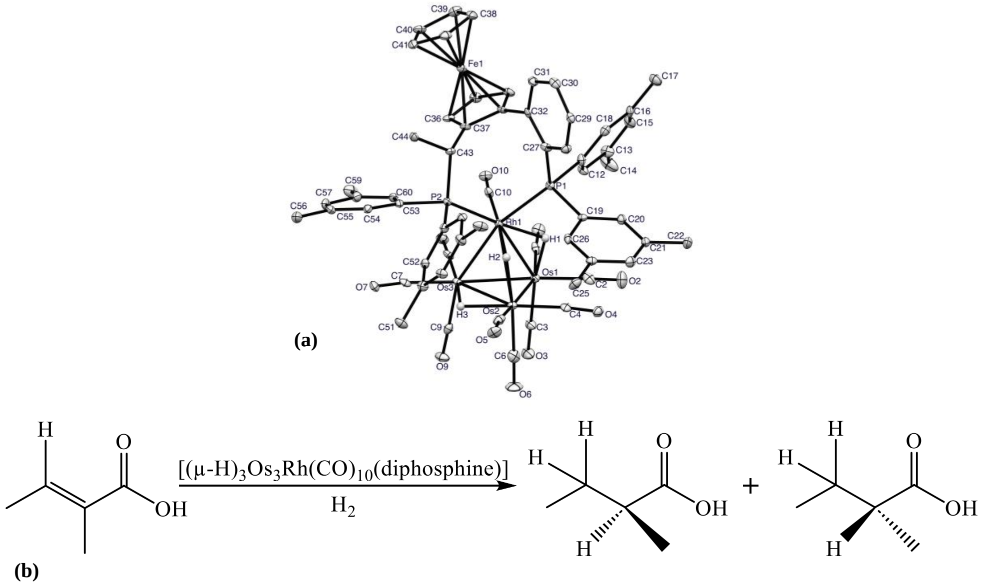

Figure 1. (a) XRD-SC structure of compound **4**; **(b)** catalytic hydrogenation of tiglic acid.

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FL09

Development of selective peptide-based radiopharmaceuticals for targeted therapy and diagnosis of high malignant cancers

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RGDechi is a bifunctional chimeric peptide composed of a cyclic RGD containing pentapeptide covalently linked by a spacer to an echistatin domain [1]. This peptide is able to selectively modulate $\alpha_V\beta_3$ function. Different properties of the RGDechi peptide have been demonstrated, such as antiangiogenic activity, antiadhesive, antiproliferative, and pro-apoptotic effects on human malignant melanoma cells.

RGDechi can be considered a great candidate as a non-invasive diagnostic tracer in tumor imaging [2]. Technetium-99m ($t_{1/2}$=6.02 h and E_γ=140 keV) is the workhorse radionuclide in Nuclear Medicine for SPECT applications.

To prepare the [^{99m}Tc]-tagged RGDechi derivative peptides the labeling approach which involved the use of the [^{99m}Tc(N)(PNPn)]$^{2+}$-system (PNP= bis-phosphino-amine) was investigated [3]. Exploiting the [^{99m}Tc(N)(PNPn)] technology, both the molecular weight and lipophilicity of the radiolabeled peptides were easily modified by varying substituents of the P atoms of PNP in [^{99m}Tc(N)(PNP)] scaffold; this allows for a fine modulation of their stability and pharmacological properties.

Take advantage of the [^{99m}Tc(N)(PNPn)] technology, a Cys residue has been coupled on the side chain of the Lys1, obtaining RGDechi-Cys analogues. A Cys residue was selected as a bifunctional chelating agent (BFCA), to allow the coordination to the [^{99m}Tc][Tc(N)(PNPn)]-synthon, through the negative sulfur (S^-) and the neutral nitrogen (NH_2) atoms affording the final monocationic complex.

The *in vitro* stabilities of the obtained radiolabeled peptides were assessed.

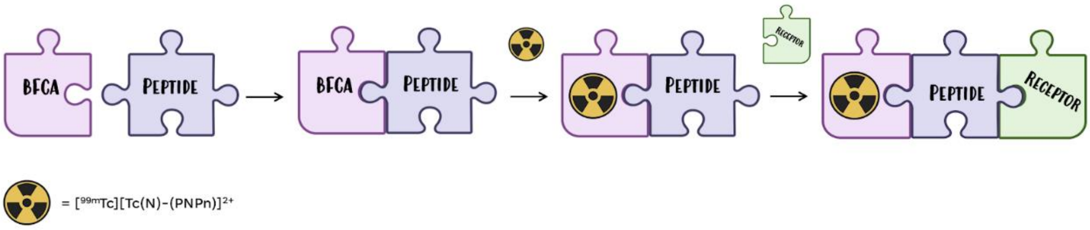

Figure 1: Schematic representation of the synthesis of BFCA-peptide, radiolabeling and the interaction with a biological target.

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FL10

Identification of new small molecules targeting olfactory receptors for the treatment of lymphoma

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Lymphomas are blood malignancies generated from lymphocytes, recurring among the ten most common cancers in developed countries. Although some progresses have been achieved along the years in increasing survival, many patients still succumb because of this disease. Hence, more efficacious approaches and better therapeutic options for refractory forms are needed. The G-protein-coupled receptors (GPCRs) play a key role in cellular physiology and homeostasis, and disruption of their pathways is associated with various diseases such as cancer. A new perspective in the treatment of lymphoma is the identification of ligands for the emerging subfamily of olfactory GPCRs (ORs), since ectopic ORs are highly expressed in different cancer tissues and their activation seems to affect cancer cell growth and progression [1]. Small molecules based on heterocyclic scaffolds constitute an important class of natural and synthetic products, widely used in the treatment of lymphoma in combination chemotherapy regimens. In particolar, overexpression, deletion or mutation of GPCRs are associated with the development of different types of non-Hodgkin's lymphomas (NHL). Tricyclic [1,2]-oxazole-based compounds, previously investigated by us, showed potent growth inhibitory effect against four different lymphoma histotypes with GI_{50} values in the low micromolar-nanomolar range [2,3]. The most sensitive cell line was found to be GCB-DLBCL (SUDHL10) expressing the GPCR olfactory receptor OR13A1. These results paved the way for the synthesis and biological evaluation of a new class of heterocyclic compounds targeting ORs.

All new derivatives were tested with the glosensor luminescence assay in the Hana3A cell line over-expressing OR13A1. Compound GSX2 emerged as an excellent ligand, showing nearly 2-fold stronger binding interaction with OR13A1 than the natural ligand cyclohexanone. On the basis of these results, iterative cycles of synthesis are ongoing to evaluate a structure-activity relationship (SAR) of the core structure with the aim to identify new candidates targeting ORs.

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[2] M. Barreca et al. *Eur. J. Med. Chem.* 243 (2022) 114744
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FL11

Does the Ala-to-Ser substitution affect the metal-binding and biological properties of the antimicrobial peptide calcitermin?

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The phenomenon of antimicrobial resistance (AMR) occurs when microorganisms become able to adapt and grow in the presence of previously effective medications. Misusing and overusing antibacterial agents are considered the major reasons behind the resistance emergence, together with spontaneous evolution and mutation of pathogens. In order to tackle this global emergence, the use of antimicrobial peptides (AMPs) represent a promising strategy for the design of new drugs. AMPs can act through different mechanisms, including the interaction with cell membranes and the innate immune response termed “nutritional immunity”. Thanks to this mechanisms, AMPs sequestrate essential metal micronutrients such as Zn(II), Cu(II), Mn(II), Fe(II), or Ca(II), which are fundamental for pathogen subsistence.

Among several AMPs, we are interested in calcitermin [1,2], a human 15 amino-acid antimicrobial peptide: VAIALKAAHYHTHKE. Calcitermin contains an effective metal binding domain with three alternated histidine residues (His 9, His 11 and His 13) and the free terminal amino and carboxyl groups. It exhibits an increased microbicide activity when Zn(II) or Cu(II) ions are present in the culture medium. In order to improve the metal binding affinity and the biologic activity of calcitermin, we synthesized and studied the analogues VAIALKSAHYHTHKE (A7S), VAIALKASHYHTHKE (A8S) and VAIALKSSHYHTHKE (A7S/A8S), in which the alanines in position 7 and/or 8 have been replaced by serines. In fact, several studies carried out on metal chelating peptides have previously shown that the presence of one or more serine residues in the proximity of coordinated histidines stabilizes the Cu^{2+} complexes when the metal ion begins to interact with the amides of the peptide chain [3]. We also studied the complexes with zinc ion, which is the most important endogenous metal ion capable to interact with calcitermin. The characterization of the complexes has been achieved by means of mass spectrometry, potentiometry, UV-Vis spectrophotometry, circular dichroism, electron paramagnetic resonance. The proteolytic stability of these three peptides has been tested in human plasma by means of HPLC, evaluating the degradation after different times of incubation at 37°C.

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FL12

Gotta oxidise them all: efficient whole-cell conversion of benzyl alcohols to acids

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Acetic acid bacteria (AAB) are Gram-negative microorganisms able to oxidise a wide variety of sugars, alcohols, and polyols with outstanding stereo- and regio- specificity, using dehydrogenases located in the periplasmic space [1]. Therefore, AAB have been thoroughly used to prepare several aldehydes and carboxylic acids, making them considerable biocatalysts in a plethora of different bioprocesses.

Interestingly, the substrate specificity and the overall oxidative efficiency strictly depends on the strains and on the reaction conditions used. In previous works, the oxidation of benzyl alcohol by different AAB strains resulted very poor [2].

Our group selected three different strains of AAB, two of them isolated from the gut microbiota of *Drosophyla suzukii,* and tested them with several aromatic alcohols, including benzyl derivatives, to broaden the substrate scope accepted by AAB.

All reactions have been performed using 1 g/L substrate using both growing and resting cells in phosphate buffer. The conversions show promising results with the majority of alcohols completely converted into their corresponding acid within 24 hours. Moreover, aldehydes can be accumulated by using a water/isooctane two-liquid phase system.

This sheds some light on a new possible industrial application of AAB for the synthesis of relevant building blocks in organic chemistry.

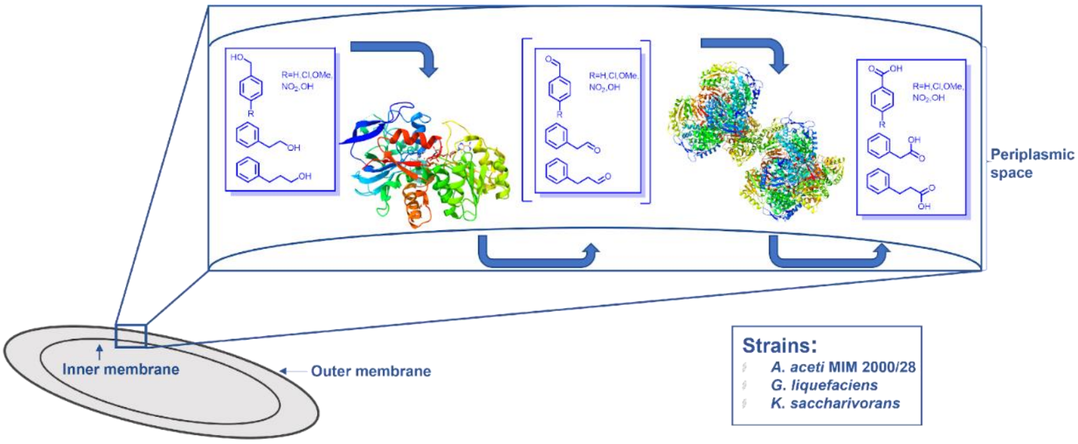

Figure 1: Substrates tested and analysed in HPLC.

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FL13

Development and analysis of glycoprotein based antiviral vaccines using mass-spectrometry

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Biopharmaceuticals currently represent the fastest growing sector of the pharmaceutical industry, mainly driven by a rapid expansion in the manufacture of recombinant protein-based drugs. Among them, vaccines represent an important class of biomolecules. Glycosylation is the most prominent post-translational modification occurring on these proteins and its specific pattern depends on the cells used for their production, such as mammalian or insect cells and yeast [1]. The aim of this project is to characterize the glycoprotein antigen glycans by using different hyphenated mass-spectrometry techniques to develop versatile analytical platforms for the rapid analysis of protein glycosylation. The settled workflows focus on three main classes of analytes originating from the glycoprotein studied: glycopeptides, glycans and monosaccharides. The analysis of the first category of molecules relies on a bottom-up proteomic approach in which the glycosites and the correspondent glycan heterogeneity and occupancy have been investigated by using tandem mass-spectrometry; the analysis of the second class of molecules occurs by glycan shaving followed by fluorescence-liquid chromatography and mass-spectrometry characterization. Finally, in monosaccharides analysis we exploit the volatility of the acetylated derivatives to analyze them by gas-chromatography. In this work we applied the listed complementary techniques to the recombinant protein gB from human cytomegalovirus (HCMV) produced in CHO cell line, which is a vaccine candidate against HCMV [2]. We describe the entire developed analytical workflow and the complete glycan characterization, which returned a deeper understanding of the product features.

Glycosylation represents a potential critical quality attribute that requires thorough analysis for a better vaccine design and to monitor product consistency [3].

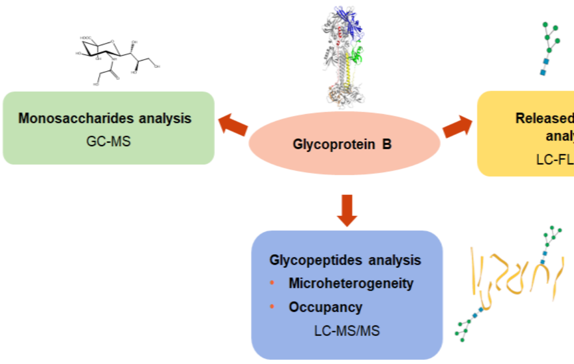

Figure 1: Schematic project view.

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[2] H.G. Burke, E.E. Heldwein, *PLoS Pathog.* 11 (2015) 1-21
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FL14

Non-covalent immunoproteasome inhibitors: virtual screening and *in vitro* test on *β1i /β5i* subunits

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Immunoproteasome inhibition is a challenging strategy for the treatment of hematological malignancies, autoimmune and inflammatory diseases [1,2]. The search for non-covalent inhibitors of the immunoproteasome *β1i/β5i* catalytic subunits could be a new strategy to avoid the drawbacks of the known covalent inhibitors. Here, we report the biological evaluation of thirty-four compounds selected from commercial libraries. A virtual screening strategy including a dynamic pharmacophore modeling approach onto the *β1i* subunit and a pharmacophore/docking approach onto the *β5i* subunit aided the identification of these hits [3]. Compound 3 is the most active onto *β1i* subunit with K_i = 11.84±1.63 µM, compound 17 showed K_i = 12.50±0.77 µM onto *β5i* subunit. Compound 2 showed inhibitory activity on both subunits (K_i = 12.53±0.18 K_i = 31.95±0.81 onto *β1i* subunit and *β5i* subunit, respectively). The hit compounds identified represent an interesting starting point for further optimization.

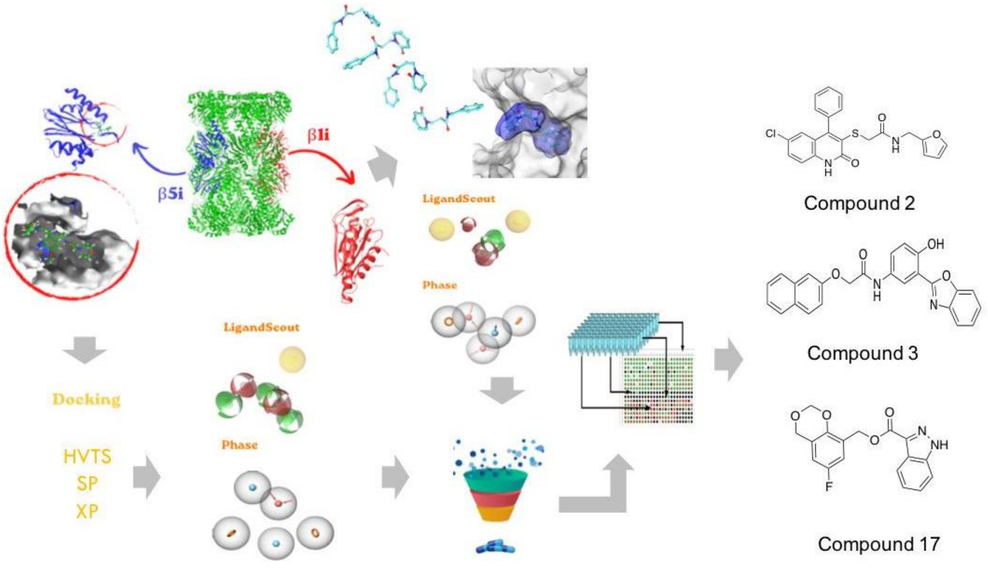

Figure1. Workflow of the study.

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FL15

A synthetic receptor for *N*-glycans: selective recognition of the core disaccharide of a sialylglycopeptide

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The recognition of specific carbohydrates on cells surfaces is well known to regulate biological and pathological processes [1]. Molecules able to modulate these processes are potentially useful both in medicine and as diagnostic tools. Among the classes of compounds capable of recognizing carbohydrates in solution, those of synthetic receptors have been deeply investigated in the last two decades. Synthetic receptors are small, abiotic compounds capable of recognizing carbohydrates by non-covalent interactions under physiological conditions. Recognition of monosaccharides is a largely explored research field, while recognition of oligosaccharides and glycans have only recently been exploited due to the complexity of these guests. In 2021 our research group proposed a new acyclic and adaptable receptor for the *N,N'*-diacetylchitobiose disaccharide ($GlcNAc_2$), core residue of *N*-glycans [2]. Given the acyclic nature of the receptor and the unprecedent affinity for $GlcNAc_2$, this molecule has the potential to tune the disaccharide inserted in a complex glycan. In the last years we have developed a second-generation receptor **1** (Figure 1) and studied, for the first time in this research field, the recognition of a disaccharide in a complex glycan [3]. The results of this study will be discussed in this communication.

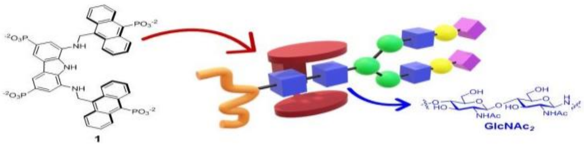

Figure 1: Receptor **1** and concept of the presented work.

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FL16

Light-tunable membrane permeability in giant unilamellar vesicles via engineering of amphiphiles

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Supramolecular structures exhibiting responsiveness to applied stimuli are a captivating area of investigation due to growing interest in systems that are capable of executing tasks based on encountered inputs [1]. Living cells serve as exemplary instance of such systems, given their unparalleled capacity to perform a wide array of activities by interacting with their surrounding environment. In this respect, there is considerable interest in reproducing these characteristics in simplified stimuli-responsive artificial systems that can be utilized as therapeutic tools (e.g., drug delivery) or for environmental purposes (*e.g.*, pollution remediation) [2].

In this work, a library of artificial amphiphiles bearing an azobenzene core was synthesized and incorporated into the bilayer of giant unilamellar vesicles (GUVs). The photo-induced *E-Z* azobenzene isomerization (Figure 1) triggered changes in the membrane morphology, leading to remarkable size and shape alterations in the GUVs. Furthermore, upon light irradiation, the formation of channels through the membrane was observed, resulting in increased permeability and the subsequent release of the contents [3].

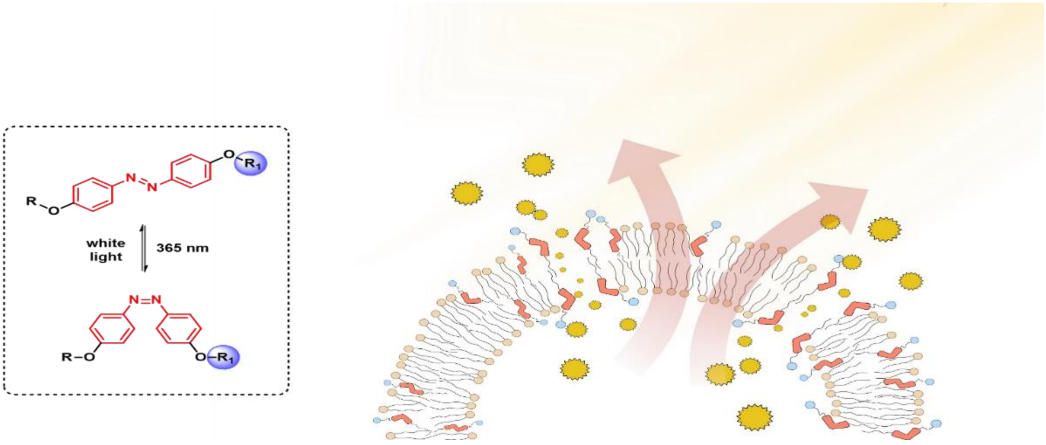

Figure 1: On the left, *E-Z* isomerization of the synthesized azobenzene-based amphiphiles; on the right, schematic picture of cargo release in the engineered GUVs.

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FL17

Novel functional elastomers based on syndiotactic propylene/α,ω-non-conjugated dienes copolymers

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Copolymers based on syndiotactic polypropylene (sPP) can be used in a wide range of applications since it is possible to tailor the physical properties of the polymer by introducing different type and content of comonomeric units in the polymer chain. Furthermore, thanks to copolymerization with suitable comonomers bearing reactive groups, it is possible to introduce different functionalities in the backbone or side groups, obtaining new materials which can be easily crosslinked or post-functionalized [1,2].

Syndiotactic copolymers of propene with different content of 1,5-hexadiene have been synthesized with a syndiospecific metallocene catalysts with the aim to introduce unsaturated functionalities in the polymer backbone. A structural and thermal characterization of all the synthesized samples has been performed to investigate the effect of the comonomeric units on the elastomeric behavior of sPP and on the polymorphic transformations occuring during deformation.

These copolymers crystallize in disordered modifications of form I of sPP, with crystallinity, melting, and glass-transition temperatures that decrease with increasing comonomer content. All copolymers show remarkable tensile properties, with great improvement of flexibility and ductility with respect to the sPP homopolymer and in particular they exhibit excellent elastic behavior.

The elastic recovery is probability related to a reversible conformational phase transition between the trans-planar form III or the trans-planar mesophase and the helical form II, which provides an enthalpic contribution to the elasticity.

The syndiotactic structure of the designed polymers ensures the development of elastomeric properties and, contemporarily, ability to crystallize. These features make the designed materials innovative smart elastomers that present, on one hand, increased stiffness with respect to conventional elastomers, thanks to the presence of non-negligible level of crystallinity, and, on the other hand, opportunities for direct and easy crosslinking and post-functionalization.

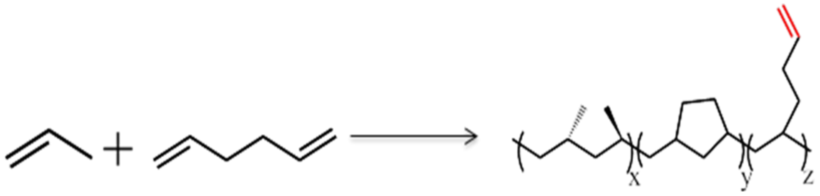

Figure 1: Scheme of the copolymerization of propylene and 1,5-hexadiene.

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[2] J N. Naga, T. Shiono, T. Ikeda, *Macromolecules* 32 (1999) 1348

FL18

New 8-trifluoromethyl-7-hydroxy-quinolinyl photoremovable protective group with potential biological applications

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Photoremovable protecting groups (PPGs) are molecular fragments that, when bound to a bioactive compound, form a biological inactive caged compound. Through irradiation with a specific wavelength, the caged compound releases the bioactive molecule allowing a spatial-temporal control over its activity. Moreover, by such a strategy, an approved drug or a fully validated active ligand can be chemically modified with different PPGs to obtain specific properties improving both biological and photochemical efficiencies. PPGs also permit the physicochemical and pharmacokinetic properties to be tuned without modifying the bioactive molecule and its biological activity [1].

The quinoline-type photoremovable protecting group allows ready release of the active molecule directly bound to heteroatoms (N, O). The compound caged by these PPGs generally has good water solubility. However, the main disadvantage of quinoline-based caged compound is that the photochemical reaction often generates several chemical species and some of them are not known yet (photobleaching) [2].

In this work, a series of quinoline based PPGs have been synthetized: 8FHQ (8-fluoro-7-hydroxy-quinolinyl), 8CF_3HQ (8-trifluoromethyl-7-hydroxy-quinolinyl), 8BHQ (8-bromo-7-hydroxy-quinolinyl) and their corresponding 7-methoxy analogues (8FMQ, 8CF_3MQ, 8BMQ). All the PPGs have been used to cage a tertiary amine and the resulting quaternary salts have been subjected to photocleavage using LED light radiation at different wavelengths: 365, 395 and 440nm. 8CF_3HQ displayed a slightly higher photocleavage efficiency compared to 8BHQ, used as a reference standard, at 365, 395 nm LED light radiation, while the other synthetised PPGs were poorly or not reactive towards light radiation. HPLC-MS studies will be performed to calculate the tertiary amine release yields and consequently assess the photobleaching effect.

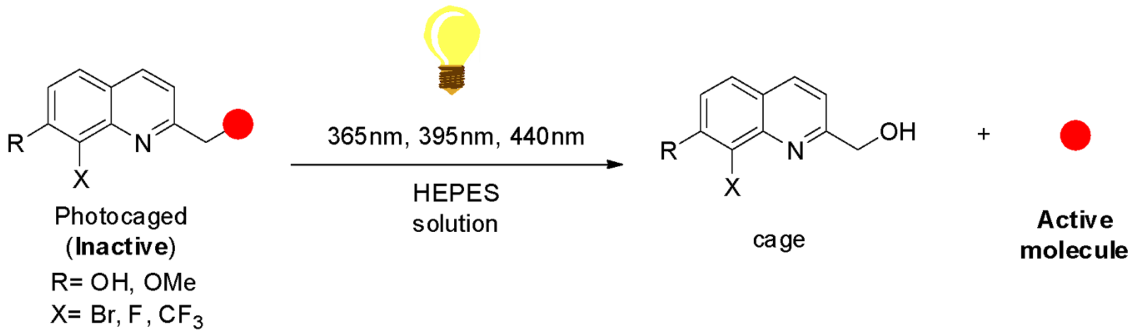

Figure 1: Photochemical reaction of the new quinoline caged compounds.

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FL19

Assessing Coulomb interactions in molecular aggregates: example applications of Frenkel’s model

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The accuracy of evaluating the UV-Vis absorption of noncovalently bound molecular aggregates relies on the distances between molecules. When intermolecular distances and molecular sizes are of similar magnitude, the conventional dipole-dipole approach becomes invalid, and at least Coulomb interactions have to be properly described. Frenkel's formalism, in which the dimer is separated into two interacting monomers, has proven to be highly effective. A recent development, integrated into the OpenMolcas package [1,2], allows for the assessment of Coulomb couplings, within Frenkel's formalism, employing multireference, multiconfigurational energetics for individual monomers, such as MS-RASPT2/SA-RASSCF. The main advantage of this method is that the computational bottleneck lies in calculating the energetics of the single interacting monomers. In this talk, I will showcase the applications of this code to dimeric aggregates of molecules with extended π systems, such as Bacteriochlorophyll (BChl)-like models or azobenzene derivatives. Various properties, including H- and J-aggregate formation and absorption spectra, will be discussed and compared to those of the isolated monomers.

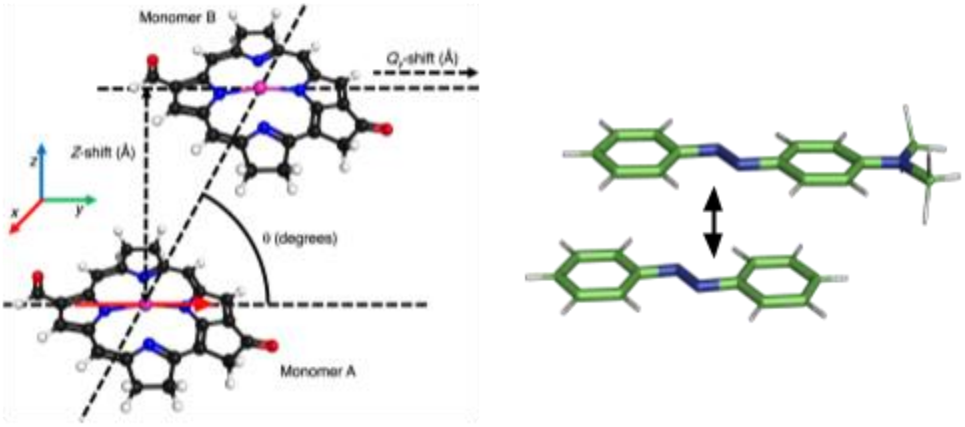

Figure 1: Homodimer model of BChl-like structures. Heterodimer model of azobenzene derivatives.

[1] A. Kaiser et al. *Journal of Chemical Theory and Computation* (2023)
[2] G. Li Manni, Giovanni, et al. *Journal of Chemical Theory and Computation* (2023)

FL20

Chemical and thermochemical approaches for sustainable energy production starting from waste biomasses

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The depletion of fossil fuels and the high pollution associated with their consumption forces the research on finding alternative and more sustainable sources. Lignocellulosic biomass has been identified as the most abundant and promising candidate for sustainable energy production [1]. In this context, the present work aims the valorisation of low-cost lignocellulosic feedstocks, as natural (*Posidonia Oceanica*) or industrial (paper mill sludge) wastes, for bio-fuel production respectively through chemical and thermochemical processes. In particular, *Posidonia Oceanica* has been chemically converted through a one-pot alcoholysis reaction for the production of alkyl levulinates, potential fuel blending additives for Diesel and/or gasoline [2]. The conversion has been carried out adopting ethanol or butanol as green reagent/reaction medium and H_2SO_4 as homogeneous catalyst obtaining ethyl levulinate and butyl levulinate, respectively. The influence of the main reaction conditions has been studied and properly tuned in order to maximize the alkyl levulinates yields.

On the other hand, the paper mill sludge, one of the most abundant waste produced by the paper industry, was investigated as possible feedstock for syngas production through the gasification process. The syngas is generally composed by CO, CO_2, H_2 and CH_4, thus it can be exploited for the production of energy (heat or electricity generation) and for the synthesis of strategic industrial compounds, such as methanol and hydrocarbons [3]. The gasification has been carried out in a fixed bed (downdraft) reactor ($\approx$100 kW_{TH}), employing a mixture of O_2/H_2O or air as gasifier agents obtaining a gas mixture of H_2 and CO of 40 vol% and 21 vol% respectively, and the characterization of the side products (tar and ashes) has also been performed. In conclusion, this work proposes the valorization of natural lignocellulosic residues and industrial wastes as low-value feedstock for the production of bio-fuels, through the direct alcoholysis treatment, or syngas, through the gasification treatment.

Acknowledgements: The authors are grateful to the European Union and Italian Ministero dell'Università e della Ricerca for the financial support provided through the PNRR project NEST. Project code PE0000021, Concession Decree No. 1561 of 11.10.2022 adopted by Ministero dell'Università e della Ricerca (MUR), (CUP I53C22001450006) Spoke n. 3 BIOENERGY & NEW BIOFUELS FOR SUSTAINABLE FUTURE

[1] S. Takkellapati, T. Li, and M. A. Gonzalez, *Clean Techn Environ Policy* 20 (2018) 1615-1630
[2] C. Antonetti, S. Gori, D. Licursi, G. Pasini, S. Frigo, M. López, J. C. Parajó, and A. M. Raspolli Galletti, *Catalysts* 10 (5) (2020) 1-22
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FL21

Reduction of formaldehyde content from special paper scraps

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Ahlstrom-Munksjo's special papers are suitable for a wide variety of applications but are mainly applied in filtration systems typically employed in the automotive sector [1]. The production of these papers is based on the impregnation of cellulose with different types of thermosetting resins, mainly phenolic and melamine-based, using formaldehyde (FA) as a curing agent. Commercially, it is essential that polymerization of the resins does not reach completion, which unfortunately causes a high FA content (>1000ppm) inside paper scraps, originating not only from unreacted FA but also from the cleavages of the polymer chains that occur randomly during the curing reaction.

FA is of concern from both a human health and environmental perspective [2], due to its toxicity and carcinogenicity. This implies that waste containing high levels of FA must be disposed of as hazardous waste (CER 15.02.02) [3], with a consequent environmental impact and higher disposal costs for the company. The goal of our work is the development of a simple and innovative treatment, either thermal or based on extraction technologies, capable of reducing the formaldehyde content below 1000ppm. Heat treatment would reduce the FA content by consuming it in the polymerization reaction, while extractive techniques would allow the extraction of unreacted FA. Once treated the waste could be disposed of as not dangerous, reducing the costs of disposal, or used as a raw material for secondary production processes.

Acknowledgements: This research acknowledges support from the project CH4.0, under the MIUR program "dipartimenti di Eccellenza 2023-2027" (CUP D13C22003520001).

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[2] List of Classifications – IARC Monographs on the Identification of Carcinogenic Hazards to Humans https://monographs.iarc.who.int/list-of-classifications (accessed 2023-04-12)
[3] Elenco dei rifiuti istituito dalla Decisione della Commissione 2000/532/CE del 3 maggio 2000, allegato D

FL22

Microwave-assisted solid-state procedure to covalently conjugate hyaluronic acid to curcumin: validation of a green synthetic protocol to prepare a biocompatible material

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Curcumin has drawn a massive interest in research devoted to investigating its employment in several disciplines, due to its wide range of biological and pharmacological activities. CUR offers outstanding medicinal properties including anticancer, antioxidant, antimicrobial, anti-inflammatory etc. The main hurdle of using curcumin for treatment of diseases is its poor solubility and lack of stability in aqueous medium.

A microwave-assisted esterification reaction [1] to prepare hyaluronan-curcumin derivatives by employing a fully solvent-free process was developed [2]. While conventional organic protocols generally rely on the efficiency of organic liquid to dissolve the reactants, herein a solid-state strategy to react two molecules characterized by a totally different solubility was developed. Hyaluronic acid, strongly hydro-soluble, was reacted with the hydrophobic curcumin, instable in water, to improve its solubility and bio-availability, while providing its own additional biological benefits (antimicrobial, anti-inflammatory, anti-oxidant, wound-repairing effects). The new protocol can be considered efficient, fast, and also eco-friendly, since it avoids toxicity and hazard in handling, such as organic base besides solvents. A cytotoxicity test confirmed that the developed HA-CUR conjugate follows the requirements for the implementation of a new material.

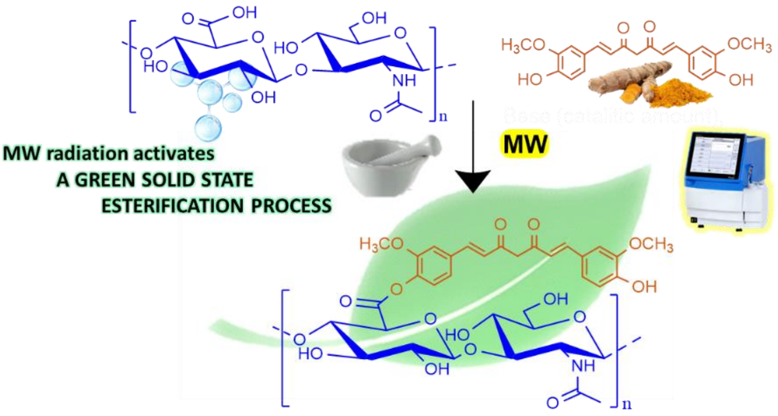

Figure 1: Chemical conjugation of hyaluronic acid to curcumin.

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FL23

Synthesis of organic dyes for water splitting in DS-PEC

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Visible-light-driven splitting of water into oxygen and hydrogen is an attractive way to convert solar energy into fuels: artificial photosynthesis and dye-sensitized photoelectrochemical cells (DS-PECs), have been deeply investigated as a promising route to convert solar energy into renewable hydrogen fuel. A crucial strategy to increase the efficiency of DS-PEC is the optimization of the dye used in the sensitization of nanostructured TiO_2 photoanode that must match with the ruthenium complex used as water oxidation catalyst (WOC) [1]. Our goal is the design, synthesis, and optimization of a metal-free sensitizer having D(donor)−π−A(acceptor) structure and photoelectrochemical properties for applicability in DS-PEC.

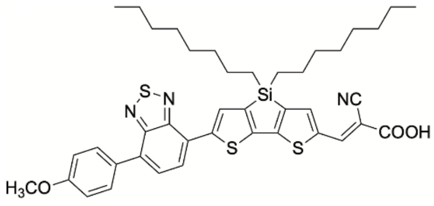

Figure 1. Structure of Dyes.

In this study, we report the synthesis of the dye **1** (Figure 1), based on a dioctyl-4H-silolo[3,2-b:4,5-b'] dithiophene central cores and having a 2-cyanoacrylic acid as acceptor group and a 4-(4-methoxyphenyl) benzo[c] [1,2,5] thiadiazol as donor group. The challenging synthesis was optimized through recent approaches as direct arylation reactions instead of common C-C bond formation by Pd-catalyzed cross coupling reactions.

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FL24

New dithieno[3,2-*b*:2',3'-*d*]pyrrole-based organic precursors of hole-transporting self-assembled monolayers for highly efficient Perovskite Solar Cells

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Thanks to the very high efficiencies in the sunlight-to-electricity conversion gained in the last ten years, Perovskite Solar Cells (PSCs) have attracted tremendous interest, stating as one of the leading technologies in the next-generation photovoltaic field [1]. Within them, the hole-transporting material (HTM), capable of transporting the holes formed after photo-excitation of the perovskite to the counter-electrode, plays an essential role in improving the performance of the device. A breakthrough has been represented by the introduction of small organic molecules as HTMs capable of forming a very thin self-assembled monolayer (SAM) [2] onto the ITO electrode and extracting the photogenerated hole from the perovskite layer.

This work aimed to design, synthesize and characterize spectroscopically and electrochemically a new family of six organic precursors of SAMs based on the tricyclic structure of the dithieno[3,2-*b*:2',3'-*d*]pyrrole and bearing a phosphonic acid as the anchoring group onto the ITO electrode. Different aryl substituents in 2- and 4-positions have been introduced to modulate the photo-electrochemical properties of the final SAMs, while a common and straightforward synthetic procedure based on Pd-catalyzed cross-coupling reactions has been optimized for all the compounds.

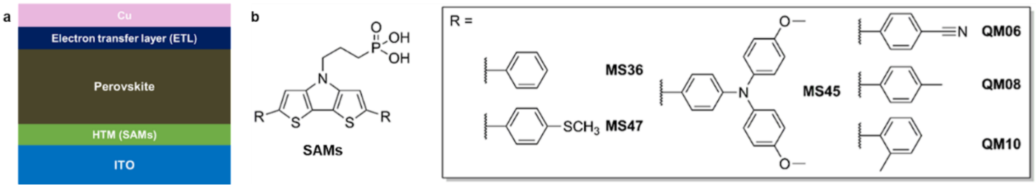

Figure 1: (a) Perovskite device structure. (b) Organic precursors of SAMs.

All the new molecules have been successfully tested for the realization of PSC devices and the most promising results have been obtained with **QM06** and **QM10**, outperforming the PCE values of the standard literature reference 2-MeOPACz [2]. Optimization of the PSC construction and full characterization of the devices is ongoing.

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FL25

In silico prediction of the organic solar cells' efficiency

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Organic solar cells (OSCs) offer significant advantages over traditional silicon devices, because of their lower costs, easier processability, improved mechanical properties, and chemically-tuneable electronic properties [1]. The identification of novel donors and acceptors boosted up the power conversion efficiency (PCE) up to 18% for bulk heterojunction (BHJ) OSC [2]; however, this value is still lower than their inorganic counterparts, thus hindering their commercialization.

Theoretical studies have the potential to play a key role in the quest for higher PCE, since determining structure-property relations can lead to the identifications and possibly the complete in-silico design of new materials with improved properties, as demonstrated by recent studies in the broad field of organic semiconductors [3]. Nevertheless, the overall OSC efficiency depends on the rates of several elementary charge transfer processes which can take place at the donor/acceptor (D/A) interface (e.g. photoinduced hole and electron transfer, excitation energy transfer, and charge recombination); thus, reliable and fast protocols for evaluating such rates from first principles are needed.

In this respect, we have developed a protocol where Fermi's Golden Rule rates for the processes occurring at the interface are computed on a reliable morphology obtained through molecular dynamics simulations, with ad-hoc parametrised force fields. We have applied this protocol over four D/A blends, representative of different ranges of efficiency and featuring different small-molecules donors and either fullerene or non-fullerene acceptors. Our results provide a simple rationalisation of the different PCE: the slower charge recombination for D/A blends with higher PCE leads to a higher ratio between charge dissociation (both via electron and hole transfer) and charge recombination rate. In light of the recently reported possibility of developing donors and acceptors with complementary absorption spectra, multiple photoexcited charge transfer pathways represent a key property to efficiently harvest the whole solar spectrum [2].

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FL26

Synthesis and characterisation of lignin-based hydrogels for the removal of emerging pollutants from wastewater

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Lignin is one of the most abundant organic polymers on Earth, exceeded only by cellulose. Lignin consists of three cross-linked aromatic units called 'lignols': coniferyl, sinapyl and paracoumaryl alcohols. Lignin has a heterogeneous structure which arises from the diversity and degree of crosslinking between these lignols [1]. Nowadays, most lignin is pyrolysed as biomass. However, new possibilities for its use have recently opened. These include its use as a component of hydrogels for the removal of drugs from wastewater due to its adsorption and retention properties of water and its pollutants [2].

Drugs have become a cause for concern worldwide as emerging contaminants for the environment. Residues of various types of drugs have been found in water. Levels of nanograms or micrograms per litre are found in water, but even at low concentrations, drugs and their residues can pose a risk to human health. Among these, diclofenac (DCF), a non-steroidal anti-inflammatory drug (NSAID), is known to inhibit the cyclooxygenase activity, and a chronic exposure to environmental diclofenac may have harmful effects on the metabolism of organisms [2].

In this study, a hydrogel LS_pAAm was synthesised from lignin sulfonate (LS) and acrylamide (AAm) by a free radical copolymerisation, using *N,N′*-Methylenebisacrylamide (MBAAm) as the crosslinking agent that enables gelation. In addition, a hydrogel with cationic functionalities (LS_pAAm_DAC) was obtained by free radical grafting with Acryloxyethyltrimethyl Ammonium Chloride (DAC) of the main chains of the copolymer LS_pAAm.

The prepared hydrogels were physico-chemical characterized and tested for the removal of the model drug DFC-Na. In the FTIR spectra, the bands corresponding to the symmetrical stretching of the $CONH_2$ amide bond and of the DAC quaternary ammonium moiety are evident. Differential Scanning Calorimetry (DSC) and Thermal Gravimetric Analysis (TGA) shows that the hydrogels are composed of 90% water by mass, and the thermal properties of the copolymers are between those of the individual units. Scanning Electron Microscopy (SEM) images show three-dimensional network structures, with regular distribution of the pores with void size ranging from a few microns to tens of microns; these pores provided channels for water transport and are beneficial to promote the diffusion of water pollutants, thereby effectively improving the adsorption effect.

The cationic hydrogel LS_pAAm_DAC has a higher swelling degree after 24 hours compared to LS_pAAm and a very good Removal Efficiency, ca. 85%.C after incubation with a 15 µg/mL aqueous solution of DCF-Na.

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FL27

Energy from waste biomass without combustion: an LCA study on a bio-fuel cell at early design stage

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Turning waste into a valuable resource is a widespread global need thanks to approaches and legislation that include the circular economy and various SDG targets [1]. Organic waste is a material stream being studied for its potential source of value-added chemicals and renewable energy. Nowadays, some techniques are present to valorize them but obtaining energy from them usually requires a combustion process.

In past research, a team from the University of Bologna developed a biofuel cell technology to be used as a treatment for waste biomass from agriculture [2]. This cell aims to enhance biomass by producing electricity, without combustion, and soil conditioner. The main advantage of this cell is that its structure can be self-produced using a 3D printer, a feature that reduces costs and increases versatility in adapting the design as needed. In addition, the developed fuel cell is portable and can process even relatively small volumes of feedstock, so it can be used at the site where the biomass originated and thus avoiding transportation to disposal facilities.

To quantify the impacts of this innovative technology and evaluate its possible optimization from an environmental perspective, this LCA study was performed.

The results showed that the impacts related to the production of the cell are already less than 10% of the total impact if the cell is used for a few hundred cycles. It was also observed that the largest impact is due to energy consumption and reagent use, particularly phosphoric acid. The environmental benefits come mainly from the recovery of phosphorus present as H_3PO_4 and to a lesser extent from energy produced and nutrients in the biomass.

Alternative scenarios were created to test different combinations of acids and bases. Nitric acid and potassium hydroxide were used instead of phosphoric acid and sodium hydroxide. The use of KOH seems promising because it adds potassium to nutrient production. Scenarios based on renewable sources (from photovoltaics) have also been explored which would lead to significant reductions in impacts. An additional model was created to test the benefits of heat recovery during the hydrolysis reaction and other energy-level optimizations. Finally, all these scenarios were compared with traditional biomass waste treatments, such as composting and anaerobic digestion including transportation impacts (at 10, 50, and 100 km). The results show that BFC technology is very promising and competitive, but also point to reduced energy consumption and nutrient recovery as the main hot spots for further improvements.

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FL28

Ammonia-production electrification: is the lithium-mediated pathway a key solution for the nitrogen electrochemical reduction reaction?

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To move a step forward to the net-zero carbon emission policy, it is essential to find a pathway combinable with renewables and complementary to the Haber-Bosch (HB) process, that causes more than 2 tons of CO_2 emitted per ton of NH_3 produced. The lithium-mediated nitrogen reduction reaction (NRR) represents the most promising electrochemical process for renewable-driven and delocalized NH_3 production. The outstanding reducing power of Li has been applied in different strategies, both continuous processes (with protons in the same cell used for N_2 activation) and in step-by-step systems.

In the latter, the formation of Li_3N is the key intermediate step. The separation of the different steps in different times or environments could allow the application of H_2O as the proton source. Indeed, the presence of a large amount of H^+ near the cathode during the electrochemical reaction (the NRR) should be avoided, otherwise the competitive H_2 evolution reaction (HER) would drastically limit the Faradaic efficiency (FE). The Li_3N formation from solid Li and gaseous N_2 is thermodynamically favored, nonetheless this specie is highly unstable and this process is nowadays the most argued by the scientific community [1].

The continuous processes have nowadays reached a FE approaching 100% [2], and an integrated process with the simultaneous H_2 oxidation reaction at the anode has also been proved in view of a scalable process [3]. This anodic reaction would be necessary to provide a controlled amount of proton in the process, and let it possible to couple NRR to H_2O splitting. However, these continuous systems are presenting some intrinsic weaknesses to be addressed, such as the organic electrolyte degradation that still limits the stability and scalability of the process.

Our laboratory is currently addressing these challenges within the SuN$_2$rise project, and an overview of electrochemical and engineering-related crucial aspects will be presented in this contribution.

This project has received funding from the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation programme (grant agreement No. 948769, project title: SuN2rise).

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FL29

Can the bacterial cytochrome *c* peroxidase from *Neisseria gonorrhoeae* detoxify peroxynitrite anion?

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Neisseria gonorrhoeae is gram-negative bacterium, which is an obligate human pathogen, being able to cause the sexual transmitted disease gonorrhoea. Since during the infection this bacterium is exposed to both endogenous and exogenous sources of oxidative stress, it possesses several defence mechanisms that can detoxify reactive oxygen species (ROS). This is very interesting from the scientific research point of view because *N. gonorrhoeae* exhibits antibiotic resistance and, to date, no vaccines against it have successfully been developed; so new drug targets are needed, and defence mechanisms are good candidates to investigate on [1].

One of the main defence mechanisms is represented by NgBCCP, a bacterial cytochrome *c* peroxidase which is classified as classical bacterial peroxidase, since it has two heme groups, a high potential E-heme and a low potential P-heme [1]. Even though the main substrate of NgBCCP is hydrogen peroxide, it has been reported in literature that human polymorphonuclear leucocytes produce nitrogen oxide, NO, during their respiratory burst, and it has also been assessed that NO can kinetically react with the superoxide radical anion, O_2^-, that is simultaneously generated by the leucocyte as well, to give rise to peroxynitrite anion, $ONOO^-$, a reactive nitrogen species with high nitrating power [2]. So, the aim of this work is to investigate the ability of NgBCCP to detoxify $ONOO^-$. Both spectrophotometric titrations and kinetic assays were performed.

After heterologously producing NgBCCP in *Escherichia coli* cells, we performed kinetic assays and determined kinetic parameters for the NgBCCP with the peroxynitrite as substrate, exploiting ABTS as artificial electron donor. We compared these data with the one for the hydrogen peroxide and we found out that both K_M and k_{cat} are of the same order of magnitude. The binding studies also show a high affinity for peroxynitrite.

In conclusion, with this work we show for the first time that peroxynitrite can be detoxified by NgBCCP, pointing out that the kinetic constants are not negligible and this interaction could play a role in further research on gonorrhea disease.

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FL30

Improving Doxorubicin cytotoxicity using light

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Doxorubicin is one of the most successful chemotherapy drugs. However, its clinical use is limited by severe side effects and the development of chemoresistance. The use of doxorubicin in combination with different photosensitizers (PSs), *i.e.* photochemotherapy (PCT), i) enhances its anticancer effect, ii) improves its delivery to tumors, iii) overcomes tumor drug resistance. Here we propose the use of doxorubicin in PCT, simultaneously acting as a chemotherapeutic agent and a PS, allowing (i) an increase in the anticancer effects of the drug, and (ii) a decrease in its dose, and thus, its dose-related adverse effects. Thanks to its extensively conjugated molecular structure belonging to the anthracycline family, we exploited the intrinsic photosensitizing properties of doxorubicin to enhance its anticancer activity in leukemia, breast, and epidermoid carcinoma cells, upon irradiation.

The ability of doxorubicin to generate reactive oxygen species (ROS), which is primarily due to enzymatic pathways, is enhanced by light activation following photophysical pathways. Photoactivation of doxorubicin generates peroxides and $^1O_2$ in a light-dependent manner. Intracellular ROS generation leads to an increase in its cytotoxic activity. We have also found that doxorubicin readily localizes in the nucleus, and after photoactivation, triggers different modalities of cell death [1].

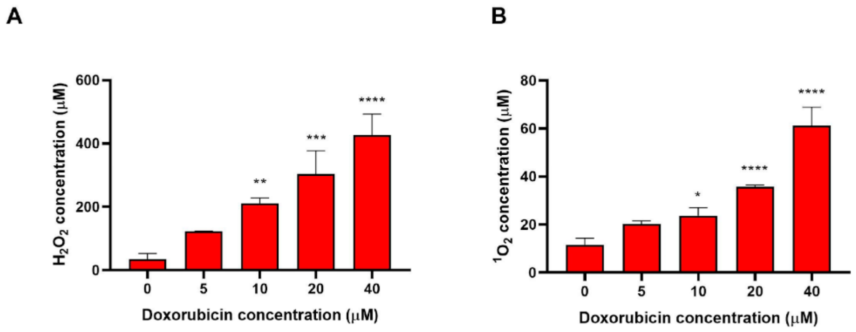

Figure 1: Quantification of ROS generated through type I (**A**) and type II (**B**) mechanisms as a function of doxorubicin concentration after 30 min of white light irradiation.

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FL31

Functionalized polythiophene based nanoparticles for efficient photoactivated therapies

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Photodynamic therapy (PDT) and photothermal therapy (PTT) are non-invasive treatments for different types of cancer. PDT and PTT rely on the use of photosensitizer agents (PS) able to generate reactive oxygen species (ROS)/heat through light irradiation to locally kill cancer cells [1].

In the realms of nanoscience and nanotechnology, thiophene-based materials play a prominent role due to their outstanding characteristics deriving from a wealth of properties such as charge conduction in the oxidized/reduced states, light absorption/emission at an appropriate wavelength, geometrical adaptability, thermal and chemical stability, and biocompatibility. Thanks to these characteristics, thiophene-based materials have been investigated as non-invasive light transduction agents, *i.e.*, systems capable of functioning as light-activated heat generators for PTT and as producers of reactive oxygen species (ROS) for PDT [2]. Herein we report the preparation of stable, biocompatible, and water dispersible nanoparticles based on a new conjugated polythiophene, able to produce heat upon irradiation. The pristine nanoparticles showed, upon laser irradiation at 808nm, the ability to reach 58°C in 1 minute, which is above the thermal ablation threshold. Furthermore, the introduction of succinimydil ester groups in the polymer structures allows the nanoparticles post-functionalization with different molecular entities - such as trifluoroethanol, fluorescein, and Rose bengal - enabling the addition of further functionalities in the resulting conjugates. This can allow the combination of photoactivated therapies within a single scaffold.

Figure 1: Schematic illustration of nanoparticles preparation and PTT experiment.

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FL32

Optimization of MEDS433 synthesis: scale-up for preclinical evaluation studies

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MEDS433, it's a novel preclinical candidate developed by the MEDSynth Research group, belongs to a novel class of *h*DHODH (*human* dihydroorotate dehydrogenase) inhibitors based on hydroxypyrazolo[1,5-a]pyridine scaffold. Extensive studies have shown its capability to induce myeloid differentiation and apoptosis in various AML (acute myeloid leukemia) cell lines, resulting in significant leukemic cell death [1]. Consequently, MEDS433 is emerging as an ideal candidate for further *in vivo* studies in AML models.

In order to conduct a comprehensive biological evaluation of the drug candidate, it was necessary to obtain significant quantities of the compound for both *in vitro* and *in vivo* efficacy, pharmacokinetic and toxicity studies. Concurrently, implementing eco-sustainable approaches in the early stages of drug development is crucial [2]. This step is necessary prior to submitting the clinical trial authorization request to regulatory agencies to prevent the need for repeating GMP evaluation and clinical trials.

This work highlights the resolution of critical issues associated with the synthesis of the drug candidate adopting greener approaches that permitted the elimination of chromatography purifications and the reduction in process waste containing by-products. Through process improvements and optimization of various steps in the synthetic scheme, a more practical and cost-effective synthesis of MEDS433 in multi-gram quantities has been achieved.

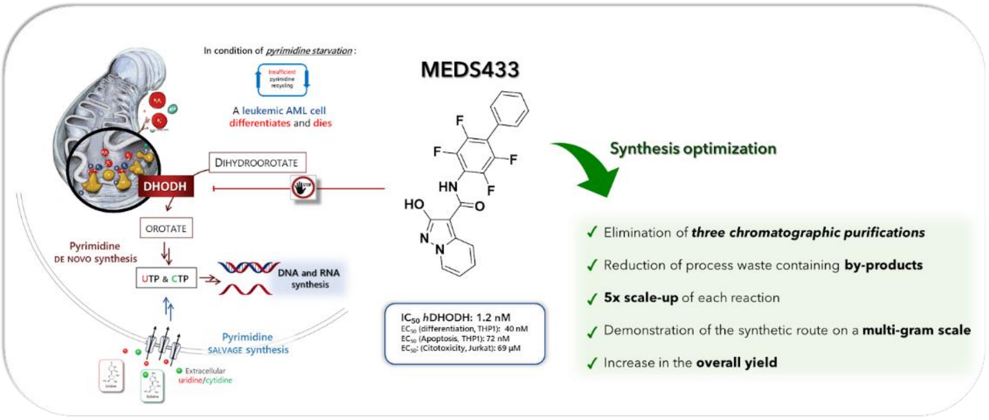

Figure 1: Key highlights of MEDS433 synthesis optimization and its biological activity on hDHODH.

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FL33

Design, synthesis and characterization of new metal chelates for novel applications as fertilizers

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Iron chlorosis is a major nutrient deficiency condition highly widespread in plants grown in calcareous soils, which leads to the development of a yellow leaf with a network of dark green veins. In severe cases, or if iron chlorosis persists over several years, individual limbs or the entire plant may die. The most common Fe chlorosis remediation technique consists in the application of iron fertilizers; however, since the synthetic processes of these complexes are dated back to the '70s, the research of innovative and optimized processes is necessary to guarantee a cheaper and more sustainable production. In collaboration with Biolchim S.p.A. we are currently focusing on improving pre-existing processes via process optimization and homogenous catalysis, while concurrently developing innovative and sustainable chelating systems able to stabilize Fe in soil solution in any condition.

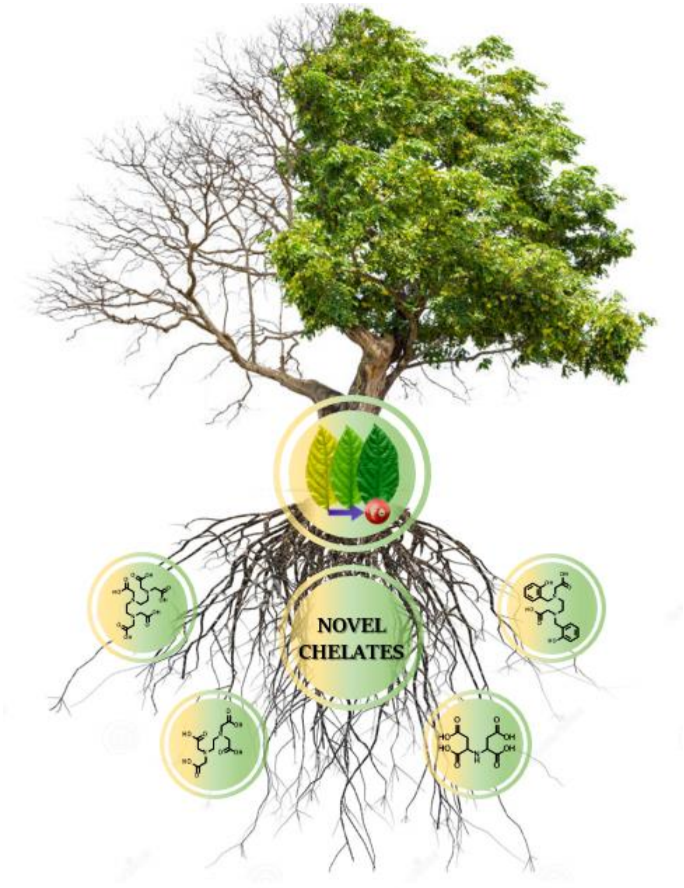

Figure 1: Fe chelates for iron chlorosis treatment.

FL34

Stimuli-responsive emulsion-based hydrogels integrated with anti-inflammatory Ozoile molecules

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In this work, we developed different types of alginate-based drug delivery system for the delivery of Ozoile. Ozoile is a pool of molecules with anti-inflammatory and regenerative properties obtained from extra virgin olive oil by a patented ozonation process [1]. Alginate is a natural polymer that is widely employed in drug delivery systems due to its numerous benefits. These advantages include easy preparation methods, biocompatibility, biodegradability, and pH-sensitivity [2]. Alginate finds application in several routes of drug administration, including targeted or localized drug delivery systems [3].

In a first step of the research work, we fabricated stimuli-responsive microspheres, responding to pH and temperature variations, for oral administration of Ozoile. For both types of microspheres, we used the electrospray technique starting from stable microemulsions obtained by high-intensity ultrasound. The microemulsions contain Ozoile at a weight percentage from 10 to 50. Poly(N-isopropylacrylamide) was used in the thermo-pH-responsive microspheres, observing a ratio of 1:1 to alginate. Next, a multilayer patch based on the alginate/Ozoile emulsion has been fabricated for use in the treatment of chronic wounds. The patch has different layers integrating various bioactive natural compounds, for example from blackcurrants, with healing and antioxidant properties. The different types of drug delivery systems were characterized using different experimental techniques, including Fourier transform infrared spectroscopy, optical microscopy, differential scanning calorimetry. Results in terms of chemical composition, pH and thermo-responsive properties, degradation behavior in physiological conditions were used to establish the potential use of the engineered systems for the therapeutic release of Ozoile at specific inflammatory sites.

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FL35

Liquid crystalline elastomers as soft stimuli-responsive actuators and support for wearable sensors

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Liquid crystal represents a state of matter intermediate between the highly ordered, anisotropic crystalline state and the isotropic liquid state. Molecules in the liquid crystalline 1phase display a certain level of order that is responsible for the specific anisotropic properties (such as optical properties, elastic modulus, viscosity). Notherless, the liquid crystalline state is highly sensitive to external stimuli such as temperature, light, electric fields that cause variations in the order parameter. The responsiveness of LCs to external stimuli makes them particularly interesting for the realization of "smart materials". For example, Liquid Crystalline Elastomers (LCEs) are unique materials that combine the responsive properties of liquid crystals and the mechanical properties of elastomers, offering the potential reversible actuation under stimuli. In the last years, our research group developed different robotic and photonic application based on these materials [1,2]. Only very recently, we focused our attention to LCE that can be used as smart supports for wearable sensors, opening to continuous monitoring of physical parameters of a patience, *e.g.* temperature or movements, in addition to the sensor operation.

Towards application as actuators and wearable smart supports, we investigate LCE prepared with different LC moieties and conditions. Through the photopolymerization of acrylate-based LCs, materials with specific molecular structure called "side-chain LCEs" were obtained. By inserting ditiohiols, that act both as chain transfer agents and chain extensors, again using acrylate-based LCs, it is possible to obtain LCE with a different molecular architecture called "main-chain LCEs". Main-chain and side-chain LCEs display very different mechanical properties and responsiveness to external stimuli.

Moreover, incorporating azobenzene molecules into the LCE matrix, it is possible to create soft actuators that can be controlled remotely and dynamically through light stimulation.

In this communication the preparation and characterization of different thermo and photoresponsive LCE will be shown towards their application as remotely controlled actuation or support for wearable devices.

N. F: acknowledge AIM (Associazione Italiana di Scienza e Tecnologia delle Macromolecole) to support his participation to this event.

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FL36

Waste recovery and valorization through alpha-hydroxylation of lanolin fatty acids mixture

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Lanolin, grease deriving from sheep wool scouring, could represent a renewable waste biomass, unique in properly said fatty acids (FAs) and, above all, alpha-hydroxy fatty acids (α-HFAs) richness. α-HFAs can be exploited in the (bio)remediation field for their surfactant and chelating ability and in the production of biodegradable polymers.

Acid components of lanolin were recovered by saponification with KOH; FAs were separated from α-HFAs benefitting of the different solubilities in organic solvents, namely methanol and cyclohexane (Figure 1A). Composition of the different portions (A-E) were assessed through ^{1}H-NMR and GC-MS [1]. After that, fractions B and E were thoroughly mixed and subjected to alpha-hydroxylation. The reaction was carried out by the production of alpha-chlorinated intermediates, using trichloroisocyanuric acid (TCCA) as a green chlorinating agent in solvent-free conditions (Figure 1B). The intermediates were eventually converted to the correspondent alpha-hydroxylated mixture through nucleophilic substitution [2]. Reaction completion was verified through GC-MS. Currently, these mixtures are studied for the realization of biopolymers.

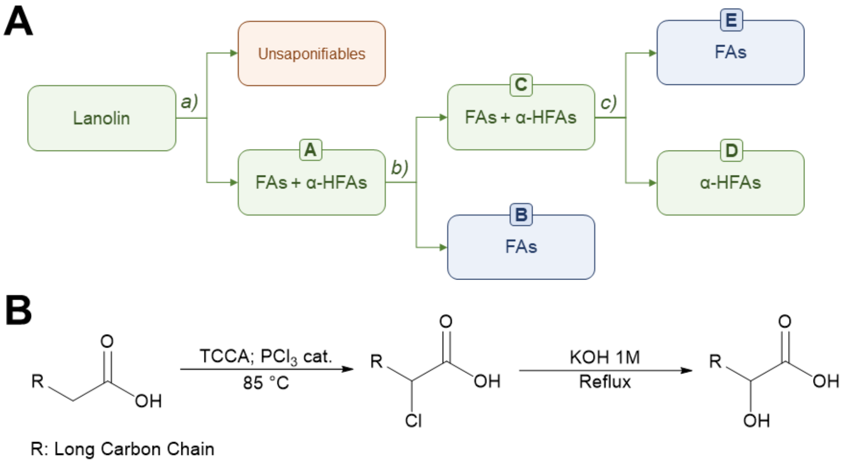

Figure 1: (Panel A) Schematic representation of lanolin acid components fractioning. *a*) KOH 10% (w/v), reflux, 48h; *b)* Methanol, rt, 2h; *c)* Cyclohexane, rt, o.n.; (Panel B) Reaction scheme for alpha-hydroxylation of fatty acids.

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FL37

Immobilization of chiral mono-amidine catalysts for stereoselective Aza-Henry reaction under heterogeneous phase

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Herein, we reported the synthesis and employment of chiral mono-amidine organocatalysts (Benz-MAM) immobilized on different supports, as efficient catalysts for the promotion of the stereoselective aza-Henry reaction under the heterogeneous phase. Benz-MAM catalysts, developed in 2011 by Johnston's group [1] provide the straightforward access, under homogeneous phase, to ß-amino nitroalkane product with enantioselection >95% starting from aryl-aldimines and aryl-nitromethanes. Notably, these substrates are valuable key-intermediates for the synthesis of Nutlin-3a, a *cis*-imidazoline anticancer agent that inhibits MDM2-p53 interaction. Although asymmetric organocatalysis is a powerful metal-free tool for the preparation of chiral molecules, chiral organocatalysts are often synthesized through expensive multistep strategies and their simply and straightforward separation and recycle are quite complex and time consuming. To overcome these problems, chiral organocatalysts can be recovered for reuse by immobilizing them to solid inert supports. For these reasons, after a study of catalytic design, Benz-MAM organocatalysts were grafted onto different supports such as: mesoporous polystyrene, mesoporous silica, polystyrene nanoparticles and hybrid silica-polystyrene nanoparticles. Once the characterization and synthetic optimization activities were concluded, the performances of the new heterogeneous catalysts were tested in the aza-Henry reaction affording the Nutlin-3a precursor in a stereoselective fashion.

Catalyst activity, stereoselectivity and recycling ability were considered as main parameters, in order to evaluate the efficiency of the novel catalytic species and speculate about their behavior

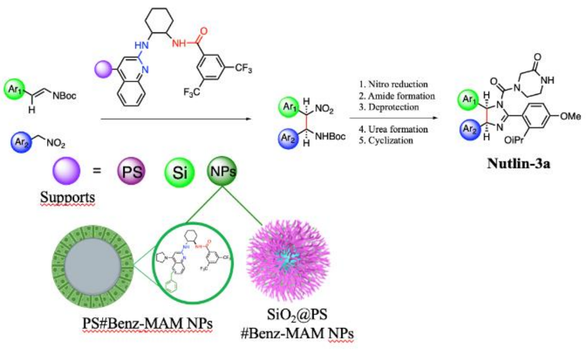

Figure 1: Immobilization of chiral mono-amidine catalysts for stereoselective Aza-Henry reaction under heterogeneous phase.

[1] B. A. Vara, A. Mayasundari, J. C. Tellis, M. W. Danneman, V. Arredondo, T. A. Davis, J. Min, K. Finch, R. K. Guy, and J. N. Johnston, *J. Org. Chem*., 79 (2014) 6913−6938

FL38

Extremely active Cp*Co(III) electrocatalysts for hydrogen production

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In recent years, there has been significant interest in the development of efficient, durable, and cost-effective catalysts for the hydrogen evolution reaction (HER) [1]. This research is motivated by the global interest in utilizing H_2 as the future energy carrier. Cobalt based electrocatalysts are viable candidates owing to their stability and relevant activity for HER [2].

Herein we report the synthesis of a series of Cp*Co(III) complexes bearing N,N and N,O bidentate ancillary ligands and their application as HER electrocatalysts in water (Figure 1). This study emphasizes the crucial role of the ancillary ligand in determining the overall catalytic performance.

Impressive turnover frequency values, up to 109,000 s^{-1}, have been observed, which rivals the performances of the best HER electrocatalysts reported to date [3]. Mechanistic studies and DFT calculations have been employed to explain the observed catalytic trends and elucidate the underlying reaction mechanism.

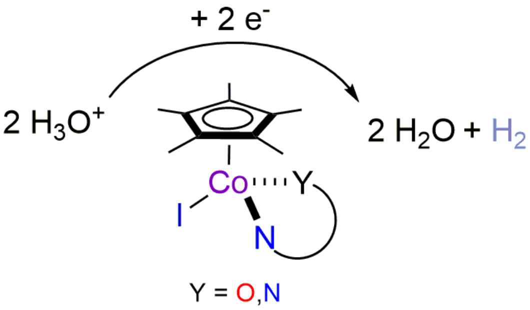

Figure 1: Electrochemical H_2 production catalysed by Cp*Co(III) complexes.

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[2] F. Zaccaria, G. Menendez Rodriguez, L. Rocchigiani and A. Macchioni, *Front. Catal*. 2 (2022), 892183
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FL39

Catalytic transfer hydrogenation of levulinate esters with ethanol over Zr-based catalysts under continuous flow conditions

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Obtaining chemicals and fuels from biomass is a key step for a sustainable development. From this prospective, cellulose is a potential source for a vast array of bioderived platform molecules, such as ethanol, levulinic acid (LA) and its easters (LE).

PRIN LEVANTE project deals with the valorization of these biobased intermediates through different strategies. A promising route is the reduction/cyclization of LE to give γ-valerolactone (GVL), an important chemical building block for organic synthesis, a green solvent, and also an additive for perfumes, foods, and fuels.

However, the reduction in liquid-phase and batch conditions involves the utilization of high-pressure molecular hydrogen (5-100 bar) in the presence of expensive noble-metal-based catalysts. In this regard, a more suitable approach consisting in the catalytic transfer hydrogenation (CTH) mediated by alcohols as H-donor has recently shown interesting results using zirconia catalyst [1]. Moreover, the reaction has proved a high conversion of LE and good selectivity of GVL under continuous flow conditions in the gas-phase by working at relative mild conditions (250°C, 1 bar) [2].

Therefore, this method was further developed and investigated by optimizing the process parameters and studying new catalytic systems. In particular, by means of the inclusion of other metals in the ZrO_2 framework, we favored the fine tuning of the catalyst' acid/base properties. This approach allowed to promote not only the consecutive reactions towards other value-added reduced compounds (Figure 1), but also to strongly reduce the deactivation rate of the material.

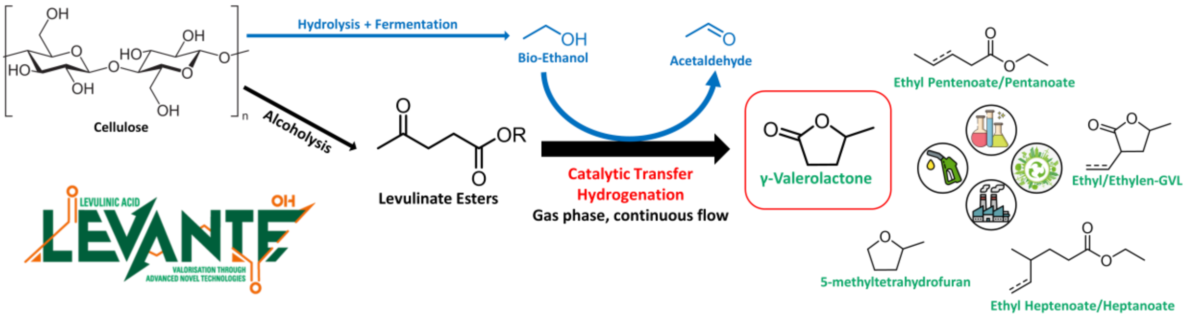

Figure 1: Catalytic transfer hydrogenantion of levulinate esters using ethanol.

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FL40

Application of untargeted UHPLC/Q-TOF-MS, GC-MS and ICP-MS techniques for new metabolites discovery of White Acqualagna truffle (*Tuber magnatum* Pico)

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White Truffle is the most expensive edible underground mushroom that grows in symbiosis with the roots of plants, and it is appreciated food for its extraordinary aroma. In this study, a first characterization of white Acqualagna truffle was carried out, due to the scarce scientific literature. The volatile profile was identified by GC-MS, and it was compared with the descriptors obtained by sensory analysis. The elemental composition was investigated through ICP-MS. To analyze the non-volatile profile of *Tuber magnatum* an untargeted metabolomics approach using an ultra-high-performance liquid chromatography coupled with quadrupole time of flight mass spectrometer (UHPLC-Q-TOF) was applied. Mass spectra were processed using MS-DIAL, which provides information about mass accuracy, isotopic pattern, and spectral matching with the library of each compound. Analysis were performed both in positive and in negative polarity acquisition modes allowing the identification of 322 and 134 potential metabolites. More than 60 compounds, in a total of 456, reported a total identification score match greater than 90%. This untargeted approach enabled the discovery of potential white truffle metabolites that have not yet been studied. The data obtained by ICP-MS analysis revealed a higher content of K, P, S, Ca and Mg, representing 97% of elements investigated. The composition of the elements between the truffles and the water released from the soils was also compared, to investigate which elements of the soil have been assimilated into the truffle.

The volatile profile consists mainly of Bis(methylthio)methane (78.72%) and other 50 minor constituents.

In conclusion, this project is the first step for the enhancement of local food, characterized by specific qualities and constituents. Furthermore, for the first time *Tuber magnatum* was characterized by non-target approach to obtain a metabolite profile.

FL41

Metabolic profiling of 100% “Datterino” tomato purees by HR-MS and identification of potential discriminant patterns

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Among fruits and vegetables, the tomato (*Solanum esculentum*) stands out for its commercial and nutritional properties. Tomato consumption either as fresh fruit or in processed products is higher than that of all other fruits and vegetables, due in part to their year-round availability and accessible prices. Tomato consumption is of great importance in the human diet, in fact it has been linked to numerous health benefits, such as decreased chronic diseases [1], thanks to its content in antioxidants and bioactive compounds, among others. Over the last decade, several metabolomic approaches using different analytical techniques have been established to identify the similarities and differences among tomato varieties [2].

The aim of the study was to provide the chemical characterization of methanolic extracts of Datterino tomato based purees, by liquid chromatography/tandem mass spectrometry (LC-MS/MS) analysis, to identify characteristic metabolites of the “Datterino” tomato purees compared to low-cost alternative commercial products with no varietal indications.

Commercial samples of tomato purees were homogenized and aliquots were extracted with methanolic solvent. After a quick extraction step (few minutes) the samples ware filtered and submitted to LC-MS/MS untargeted analysis for the metabolites profiling. The raw data were processed by Compound Discoverer v.3.3SP1 (Thermo Fisher Scientific) and identification was accomplished by ChemSpider and mzCloud nodes, namely according to the accurate mass of the precursor ions and their characteristics fragmentation pattern, respectively.

The metabolic profiles of tomato purees were collected confirming the presence of nutritionally relevant compounds. The typical patterns were defined and main metabolites classified according to their structural characteristics (e.g. phenolic alcohols, organic acids, amino acids, etc…). Finally, a preliminary investigation about the identification of potential discriminant patterns of authentic Datterino tomato-based puree was carried out and the perspective application of this analytical approach will be critically discussed.

Acknowledgements: This research was funded by AGRITECH- Centro Nazionale di Ricerca per le Tecnologie dell’Agricoltura, PNRR MUR-M4C2 (Missione 4 Componente 2) Investimento 1.4 “National research Centre for Agricultural Technologies” Agritech CUP HUB – B63D21015240004.

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FL42

A feasible 7-step synthesis of 7-hydroxy cannabidiol

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7-Hydroxy-cannabidiol is a primary metabolite generated during the first stage of cannabidiol metabolism. Cannabidiol is one of the most abundant phitocannabinoid obtained from Cannabis sativa and it is well known because of its non-psychotic activity and its pharmacological activity as an analgesic, antibacterial or anti-inflammatory but also shown therapeutic activity related to neurological disease such as epilepsy [1]. Since 2018 the European Medicines Agency (EMA) has approved the first cannabidiol-based drug in pure form for the treatment of two severe forms of drug-resistant childhood epilepsy or its intake in combination with commonly used antiepileptic drugs.

Since the underlying mechanism by which cannabidiol exert its therapeutic efficacy has not been fully elucidated it is plausible to think that some of the effects observed could be attributed to active metabolites. For this reason, 7-hydroxy-cannabidiol is particularly attractive as a potentially biologically active metabolite. To date its use is purely as a reference standard in analytical methods aimed at elucidating the pharmacokinetics of cannabidiol. But the future of research in this field could change if its biological activity is confirmed. To achieve this goal, it is desirable to develop a robust synthetic protocol to allows preclinical and clinical studies on this specific substance. To the best of our knowledge scientific literature reports only a dedicated eight-steps synthetic pathway from cannabidiol, which involves a critical step that makes use of hazardous reagents [2]. In this project it is presented a seven-steps synthesis with two one-pot procedures starting from commercially available cannabidiol. The developed methodology requires milder and safer reaction conditions avoiding the use of dangerous chemicals. The innovation lies in being able to circumvent the critical issues relating to the substrates avoiding hazardous working conditions for the operator. The synthetic protocol was performed in small to medium scale with overall yields of 18 to 31% of desired product.

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Poster presentations

POS1 - ASTOLFI Eleonora (UniBO)

POS2 - BELLINA Francesco (IIT)

POS3 - BRAIDO Rachele (UniVE)

POS4 - D’EUSANIO Veronica (UniMORE)

POS5 - DE ROSA Teresa (UniNA)

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POS68 – PAN Wenkai (UniBO)

POS69 – TORTORELLA Sara (Molecular Horizon)

POS1

Metal Organic Frameworks as electrocatalyst for the electrochemical CO_2 conversion

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Dipartimento di Chimica “Giacomo Ciamician”, Alma Mater Studiorum – Università di Bologna, Via Selmi, 2, 40126 Bologna (BO), Italy

The resulting accumulation of the industrial greenhouse gas CO_2 in the atmosphere is the primary driver of today’s climate change [4]. Anthropogenic CO_2 is released in the biosphere at a rate of 34 Gt per year and only 0,6% is currently recycled [3]. In the biological metabolism, reduction of CO_2 in photosynthesis balances the oxidation of carbon in cellular respiration, carbon reduction is yet a missing piece of humanity’s industrial metabolism. This imbalance has become a perturbation to Earth’s natural carbon cycle. Strategies to reduce net CO_2 emissions fall under three categories: decarbonization, carbon sequestration, and carbon recycling, all three of which will need to play a role *(Figure 1).* [4]

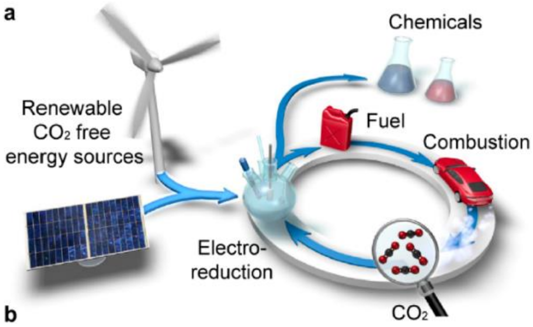

***Figure 3**. Electrochemical reduction of CO_2 coupled to renewable electricity sources, such as wind or solar, can potentially enable a CO2- neutral energy cycle in which CO_2 is converted to fuels and industrial chemicals in a renewable and sustainable manner.[2]*

Direct use of CO_2 via electrochemical reduction of CO_2 (CO_2RR) presents a means to obtain high-value products and concomitantly offset CO_2 emissions [1]. The main problem of the reaction is due to the thermodynamic stability of CO_2 whose standard formation enthalpy is -393.5 $kJmol^{-1}$. My thesis’ project is an interdisciplinary one that investigate both the synthesis and characterization methods of copper-based Metal Organic Frameworks (MOFs) used as molecular electrocatalyst deposited on GDE for CO_2 reduction to obtain value-added products or fuels.

Three fields of chemistry are merged to achieve this aim:
(i)Organic chemistry for the synthesis and characterization of the coordinating ligand of Cu^{2+},
(ii)Inorganic chemistry for the synthesis and characterization of the Cu^{2+} based MOF,
(iii)Electrochemistry to evaluate the applicability of the innovative material in the CO_2 valorisation to provide sustainable energy requirement. The electrochemical reduction of CO_2 is studied at different potential values.

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[3] ACS Energy Lett. 2016, 1, 281−282
[4] Chem. Rev. 2019, 119, 7610−7672

[3] ACS Energy Lett. 2016, 1, 281−282
[4] Chem. Rev. 2019, 119, 7610−7672

POS2

Study and development of new RNA targeted probes

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Within D3-PharmaChemistry group at IIT, we are aiming to possibly identify novel small-molecule modulators targeting non-coding RNAs (ncRNA). Specifically, our primary objective is to discover small molecules able to modulate the microRNA-21 (miR-21), whose overexpression is involved in cancer and tumorigenesis process [1]. The idea is to identify compounds belonging to a new chemotype able to inhibit the interaction between miR-21 precursor (pre-miRNA-21) and its cleavage enzyme (Dicer), thus decreasing the formation of the mature miR-21. In our project, we initially performed a high-throughput screening (HTS) against pre-miRNA-21; following, among the initial identified hits, we mainly invested our efforts in the synthetic evolution of compounds featuring a substituted 4-pyrazolyl cyclopenten-1-amine scaffold, which showed promising preliminary selectivity and activity (K_d) in the low µM range for pre-miRNA-21. To pursue our efforts, we envisaged a synthetic strategy taking advantage of an *ad hoc* developed Heck-Matsuda reaction [2] employing substituted pyrazolyl-derived diazonium tetrafluoroborate salts, which allowed to stereoselectively confirm the hit's structure, and produce a series of close, promising analogues. (Figure 1). Starting from the HTS hit, the chemical evolution within this series led to more than 40 analogues featuring various modifications in most relevant structural portions of the hit's core scaffold. The affinity toward the target primarily stirred the structure-activity relationship to design novel analogues. Considering the data of the initial hit (K_d= 0.501 ± 0.19 µM), our exploration has led to compounds with a significantly improved affinity in the low nM range. The project is still on going and in the following months, we will focus on further investigating the most promising compounds trying to evaluate their inhibitory activity towards the hydrolysing enzyme Dicer. In the last months, I have started to build a new molecular dynamic–based binding model which could help us designing new analogues and eventually develop de-novo ligands for the target.

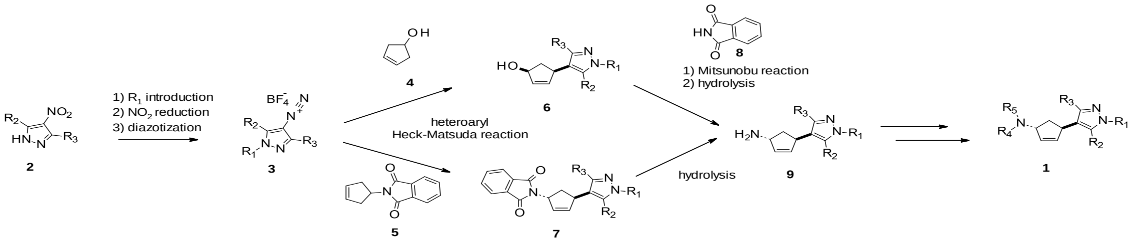

Figure 1: Synthesis of substituted 4-pyrazolyl-cyclopenten-1-amines **1**.

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POS3

A study on catalyst's structure: $Ni@Al_2O_3$ core-shell for Dry Reforming of Methane

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The process of simultaneous conversion of CH_4 and CO_2 to obtain syngas (CO and H_2) is known as Dry Reforming of Methane (DRM). The DRM reaction is receiving considerable attention because it enters in the field of carbon capture utilization (CCU). In fact, DRM is a powerful way to transform GHGs into syngas, converting its production in a more sustainable perspective. The reaction is strongly endothermic so it requires high temperatures, as well as an efficient catalytic system in terms of activity and stability.

In recent decades, many studies have been focused on catalysts based on noble and not noble metals like Co and Ni, which demonstrated activity comparable to that of noble ones. Furthermore, different types of oxides have been used as catalytic support, such as SiO_2, CeO_2, ZrO_2, La_2O_3 and Al_2O_3.

However, despite the latest advances, the reaction is not yet applied at industrial level due to easy deactivation of the catalytic systems, in particular the ones based on Ni. This because of two reasons: coke deposition, formed by secondary reactions, and sinterization of active phase, due to the high temperatures required.

To solve this, in the catalytic system can be introduced promoters such as Fe, Ce, V or the design of the catalytic system can be improved [1,2].

As concern Ni on alumina, that is the industrial catalysts for this type of reactions, a suitable and not so studied structure is the core shell one. In fact, is reported that this kind of structure should be more resistant to coke deposition and Ni sinterization [3].

The aim of this work is the study of $Ni@Al_2O_3$ core-shell catalyst. Its characteristics were investigated and compared with other catalytic systems, synthetized with different methodologies (for example by coprecipitation).

The catalysts obtained were tested for the DRM reaction at 650°C in a fixed bed reactor with a GHSV of 12000 h^{-1}, using a $CH_4/CO_2/He$ reagents mixture 1:1:18, under a total flow of 200 mL/min.

The fresh and spent catalysts were characterized, using various techniques, including: XRD, SEM, TEM, TPR, TPO, nitrogen physisorption.

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[3] J. Pu, K. Nishikado, N. Wang, T. T. Nguyen, T. Maki, and E. W. Qian, *Appl. Catal. B: Environ*, 224 (2018).

POS4

Investigating the potential of vine pruning chips for non-structural lightweight concrete in the context of sustainable development

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This study explores the utilization of grapevine pruning chips as a sustainable aggregate for producing lightweight concrete with thermal insulation properties.

The research aligns with the principles of circular economy, sustainable development, and the pursuit of the United Nations' Agenda 2030 goals [1]. Lightweight concrete has gained significant attention in the field of bioconstruction due to its numerous advantages in terms of sustainability, energy efficiency, and environmental impact [2]. Unlike traditional concrete, which is dense and heavy, lightweight concrete incorporates lightweight aggregates that reduce its density while maintaining its structural integrity.

The experimental investigation focused on examining the mechanical strength and thermal conductivity of the lightweight concrete made with grapevine pruning chips. The chips were roasted at different temperatures (120, 160, 200 and 240 °C), and the variation of concrete characteristics as a function of the pre-treatment was evaluated. Furthermore, the effect of the wood content on the concrete's performance was assessed. To evaluate the performance of the lightweight concrete, flexural and compressive strength tests were conducted, providing insights into its structural integrity under different loading conditions. Additionally, thermal conductivity measurements were carried out to assess the material's heat transfer characteristics.

The results indicated that the inclusion of vine pruning chips led to a reduction in the overall density of the concrete, resulting in a lightweight material (< 800 kg/m^3). Furthermore, as the organic material content increased, the concrete exhibited improved thermal insulation properties. The roasting temperature also influenced the final properties of the concrete, with higher temperatures leading to enhanced performance, particularly the compressive strength (from 2MPa of the specimens made with chips roasted at 120 °C to 3.5MPa of the specimens made with chips roasted at 240 °C).

By incorporating vine pruning chips into concrete production, this study demonstrates a sustainable approach to waste management while simultaneously contributing to the development of environmentally friendly building materials.

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[2] Thianel, KC, Haller T., Beuntner N. Lightweight Concrete – From Basic to Innovations. *Materials* **2020**, 13, 5, 1120. https://doi.org/10.3390/ma13051120

POS5

Monitoring of cyanobacterial blooms along the Campania coastline: anabaenopeptins detection in the food chain

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Cyanobacteria of marine origin are one of the sources of greatest interest for their function as bio-indicators of environmental health status due to their physiological adaptability that allows them to colonize different habitats and to adapt to different environmental stressors. Under conditions of excess nutrients (eutrophication), cyanobacteria proliferate to form blooms on the water surface, which are an environmental and food concern due to the production of toxic secondary metabolites, known as cyanotoxins, that can cause adverse effects on human health as well by entering the food chain through contamination of marine organisms. [1].

Therefore, constant monitoring is what we have been doing for years to identify the presence of cyanobacteria and their toxins in coastal waters of the Campania region, South Italy, to provide early warning of a cyanobacterial bloom event through our multidisciplinary strategy, named 'Fast Detection Strategy' (FDS), based on combined proximal/remote sensing and MS-based molecular networking [2,3].

In particular, the monitoring project led to the detection of the cyanobacterium Planktothrix rubescens and the rapid identification of the cyanotoxins Anabaenopeptin A and B for the first time in the crude extracts of the bivalves samples collected in the waters of the Lucrino Sea, Naples. This discovery came because of the Planktothrix rubescens bloom in Lake Avernus, Naples, during the early spring of 2022, which turned the lake red for a few days and whose contaminated waters then overflowed into the Lucrino Sea through the outlet of its channel.

The result of this research should then confirm the usefulness of cyanobacterial blooms and their toxic secondary metabolites as bio-indicators of the degree of water quality in coastal ecosystems and the effectiveness of our multidisciplinary monitoring protocol to provide early warning of a bloom event and to detect cyanotoxins without the need for long and complex chromatographic purification.

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POS6

Visible light-driven amides's synthesis via acyl chloride

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Visible light-driven organic reactions have evolved and represent a method widely used in organic synthesis. For these reasons the interest in the development of friendly green chemical synthesis has increased. We have focused our study on the development of new photocatalyst based on earth abundant metal salts instead of rare and extremely expensive Ru (II) and Ir (III) complexes [1][2]. This work reports an amidation of aldehydes via acyl chloride catalyzed by $FeSO_4$, using NaCl as chlorine source, and under visible-light irradiation. The methodology can be performed using sunlight or artificial visible light as solar simulator or blue LED source (Figure 1). Reactions were carried out starting from non-conventional starting material to obtain compounds with high-added value. Moreover, use of visible light as energy source can lead to new reactivity modes in organic reactions and it is considered safety, sustainable and accessible. These considerations pointed out how a photosynthetic method is very appealing from an ecological point of view [3].

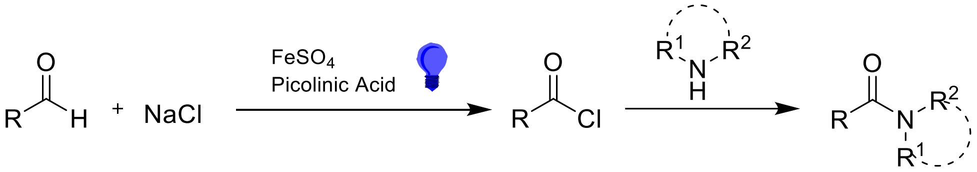

Figure 1: Amidation of aldehydes.

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POS7

X-ray diffraction study of strain Induced crystallization of hydrogenated nitrile butadiene rubbers: effect of crosslink density

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The mechanical properties and the structure of commercial samples of hydrogenated acrylonitrile-butadiene rubbers (HNBRs) are investigated. The analysis is focused on samples with acrylonitrile units (ACN) and residual double bonds content of 44 wt% and 9 %, respectively, and different crosslink density. The properties of the vulcanized samples are compared with those of the uncured one. All the samples are amorphous at room temperature and show glass transition temperatures that increase with increase of the crosslinking density. The values of the Young's modulus of the vulcanized samples are similar and three times higher than that of the uncured counterpart. The tensile resistance, instead, increases with increasing the crosslink density, whereas the deformation at break decreases. All the samples are amorphous at low deformations, but whereas the uncured and the weakly and medium crosslinked samples undergo strain induced crystallization (SIC) above a critical value of deformation, the highly crosslinked samples break at deformations close to the SIC onset. The degree of orientation of the amorphous phase gradually increases with an increase of deformation and for the samples undergoing SIC, it reaches a plateau at crystallization onset. For these samples the onset of crystallization is associated with a relaxation of the amorphous chains connected to the crystallite stems, as it is predicted by the Flory theory. The remarkable tensile strength of the crystallizing HNBRs at high deformation is attributed to the high alignment of crystals formed by SIC in the stretching direction that strengthens the materials and causes strain hardening.

POS8

Perovskites for CO_2 valorization

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Carbon dioxide is an abundant greenhouse gas accounting for 79% of global warming. In order to reduce its concentration, it is important to implement strategies such as the conversion into high value-added products such as fuels and chemicals [1]. Methane is a product of high interest, as it is the main component of natural gas and can be exploited and used as an energy source in industrial plants, in residential heating, and as fuel in automotive. It is also a building block for the synthesis of various chemical compounds, such as olefins, methanol, and syngas [2]. Due to carbon dioxide inertness and low reactivity, additional energy is required for its activation. Photocatalysis, specifically CO_2 photoreduction with water vapor, is an alternative catalytic approach, which exploits solar energy as an abundant, unlimited, renewable energy source, and enhance carbon dioxide conversion into different solar fuels, without requiring additional energy input to make the reaction take place.

Titania is the most used semiconductor in photocatalysis as it is non-toxic, available, economical, stable and has a high photocatalytic activity; however, its use is limited because of high bandgap of about 3.2 eV, that allows the absorption of radiation only in the ultraviolet region, sensibility to surface's degradation, and high recombination rate. For this reason, it is necessary to develop novel photocatalytic materials that prevent or minimize these problems. The aim of my research is the study of perovskites such as $BaTiO_3$ and $CaTiO_3$ that are gaining attention, in virtue of the good photostability, corrosion resistance, photocatalytic properties and the intrinsic basicity given by the barium and calcium ions, which favor the interaction with carbon dioxide [3]. Therefore, the catalysts were synthetized by the hydrothermal method. In addition, nitrogen and carbon were doped to perovskites aiming to exploit the full sunlight spectrum and increase the light absorption range of the selected catalysts. This could permit to introduce new intra-gap energy levels, so that the electrons could be deflected and do not return to the valence band. All the materials were characterized through FT-IR, DRS, SEM-EDX, TEM, N_2 physisorption, and XRD techniques and then tested in both gas and liquid phase under both solar and UV light to correlate their photoactivities with their physical, chemical, and optical properties.

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POS9

SuN2rise: the ERC-StG project targeting photovoltaic-driven electrochemical nitrogen fixation for ammonia refinery

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The preservation of our planet is the most urgent issue in the world and the scientific community is pushing a lot of researchers to work on technologies for the storage/conversion of CO2 into chemicals. However, it is easier not to produce CO2 than setting-up plants to treat it.

In this framework, the ERC-StG project SuN2rise proposes an alternative breakthrough based on a versatile solar-driven strategy leading to redesign industrial processes. Facing the Haber-Bosch process for ammonia production (one of the most impactful chemical processes today), we propose the electrochemical fixation of dinitrogen into ammonia, by simply using air, water and ambient conditions. The scientific aim is that of demonstrating an integrated device where a photovoltaic (PV) unit will power a regenerative electrocatalytic cell converting dinitrogen to ammonia (E-NRR). A newly proposed Li-mediated approach under mild conditions, derived from an interdisciplinary contamination between electrocatalysis and Li-batteries, will be the key towards N2 conversion, bypassing both the competitive hydrogen reduction reaction and the complete irreproducibility of recent E-NRR approaches attributed to N-contaminations or degradation of N-based catalysts.

The team will further move beyond the state-of-the-art by fabricating transparent devices, that can be integrated in greenhouses, allowing the production of ammonia and ammonium fertilizers directly in farms, bypassing the known issues related to the massive infrastructure of ammonia plants and difficulties in reaching remote communities. The proposed approach will significantly impact also the field of liquid fuels, being ammonia safer and with higher energy density than hydrogen. Achieving these goals will require multidisciplinary expertise in the field of chemical, material, process and device engineering.

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No. 948769, project title: SuN$_2$rise).

POS10

Electrocatalytic materials and devices for the water splitting

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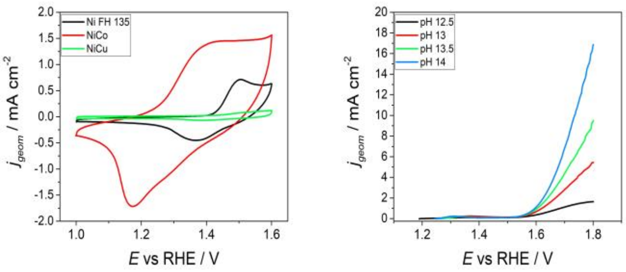
Electrolytic water splitting to generate hydrogen and oxygen is one of the most promising ways to harness intermittent renewable power sources, store the provided energy as a clean-burning and sustainable fuel and mitigate greenhouse gas emissions. However, in the water splitting reaction, constituted by the hydrogen evolution reaction (HER) at the cathode and the oxygen evolution reaction (OER) at the anode, the HER rate is often limited by that of OER due to the more sluggish kinetics and the large overpotential of the latter, which lowers the overall energy conversion efficiency.In this context, nanostructured catalysts have emerged as a promising avenue to address these limitations. Precious metals, such as Pt and Ir, have demonstrated excellent catalytic activity for the OER and HER. However, their widespread implementation for large-scale hydrogen production is mainly hindered by their high cost and limited availability. This master thesis fits into a larger research project, focused on the study and characterization of nanostructured electrocatalysts for the OER, based on non-precious metals such as Ni, Co or Cu, at different pH values, aiming to elucidate the pH-dependent catalytic behaviour [1][2]. Electrochemical techniques such as cyclic voltammetry (Graph 1), linear sweep voltammetries (Graph 2) and electrochemical impedance spectroscopy have been used for catalyst activation, oxygen production and ohmic drop corrections.



Graph 1 and 2: Cyclic Voltammetries of Ni(np)/C, NiCo(np)/C and NiCu(np)/C catalysts in Ar-saturated KOH 0.1M electrolyte (left); Linear Sweep Voltammetries of NiCo(np)/C catalyst at different pH values (right)

The collected data have been rationalized by comparing each catalyst's measured anodic current as a function of pH, by quantifying the produced oxygen and by calculating the electrochemical active surface area. Overall, this research has the potential to enhance the understanding of the underlying pH dependent OER mechanism, paving the way for the design of more efficient and sustainable electrochemical devices for hydrogen production.

We thank Ferdinand Hof for the synthesis of the graphene-supported nanostructured electrocatalysts used in this project.

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POS11

Effect of annealing on polyethylene pure grades and corresponding blends intended for biaxially stretching process

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The identification of an efficient recycling strategy in plastic packaging sector is hampered by the fact that polyolefins, like polyethylene (PE) and polypropylene (PP), are often combined in multilayer films in which different materials are glued together. To promote circularity of the plastics economy it is mandatory to improve separation and reprocessing technologies. Proposing mono-material laminates, entirely based on PE, may represent a proper solution.

The concept is to improve PE-based films properties, such as mechanical, optical and barrier properties, via biaxial stretching [1]. To establish a clear correlation between the chain microstructure, the crystalline microstructure, in terms of crystalline and amorphous phase arrangement, crystalline structure and the final properties in biaxially oriented PEs (BOPEs) it's required to perform a comprehensive characterization of PE pure grades and blends.

Tentering process is a sequential or simultaneous process in which the polymer melt is first melt extruded onto a cast roll, and then stretched sequentially or simultaneously in the 'machine direction' (MD) and the 'transverse direction' (TD) and is usually conducted in semi-solid state.

To understand the effect of temperature and time in the early stage of the tentering process, a thermal protocol has been set; each sample is:

1. heated and kept to a maximum temperature T_{max}, to ensure the erasing of thermal and mechanical history.
2. quickly cooled to room temperature.
3. fastly heated to a second temperature, $T_{annealing}$, and kept at this temperature for a certain time.
4. fastly cooled to room temperature again

The cycle is repeated for different times, choosing Tannealing within a processability window (110-130°C) selected from industrial experience.

This protocol has been applied to DSC, SAXS and POM analysis to observe what happens in the first 300 s at processing T at different length scale and eventually to determine which is the time scale of these changes.

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POS12

Smart nanomaterials with potential antibiofilm activity for medical devices

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Antibiotic resistance is a serious public health problem. Bacteria can self-produce a polymeric complex architectural structure called *biofilm*. Wrapped by this structure they become much more resistant to antimicrobial treatments, harsh environmental conditions, and the host immune system. Conventional antibiotic drugs are unfortunately inadequate to eradicate biofilm-mediated infections. In addition, biofilm infections on medical implants such as valves, stents and catheters require their surgical removal and replacement, and recurrences of infection are very high. [1] There is therefore an urgent need for materials that prevent bacterial biofilm formation to make medical devices for hospital use. Simultaneously with this, the world is facing another serious environmental and ecological problem resulting from the overuse of chemicals and petroleum-based materials. [2] Our goal is to make a smart multilayer material to cover biliary catheters, often obstructed by biofilm-type infections, based on nanocellulose, a nanomaterial extracted from renewable biomasses. On a plastic surface we laid two layers of nanocellulose on top of each other. The first was cationic nanocellulose functionalized with quaternary ammonium groups, and the second was anionic decorated with Ag Nps, known in their literature for their anti-biofilm properties. A fluorescent marker was added to the various layers to allow them to be characterized by confocal microscopy. Our future goal the selection of other layers of nanocellulose further decorated with agents with known anti-biofilm activity and to produce a three-dimensional model to better verify the antimicrobial activity of the material and its resistance to bile flow.

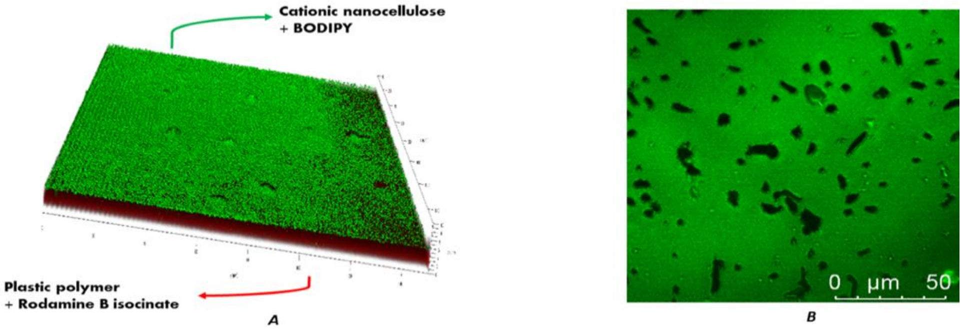

Figure 1: Confocal Microscope Images. ***A*** Double layer: labeled plastic polymer and positive labeled nanocellulose layer. ***B*** Triple layer: unlabeled plastic polymer, unlabeled positive cellulose, and labeled negative cellulose decorated with Ag Nps evident in the image.

[1] Li, X. H., & Lee, J. H. *Journal of Microbiology* (2017),55, 753–766
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POS13

An easily customizable glyconanomaterial with biomolecular recognition properties

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The development of reliable custom nanomaterials for precision medicine applications is a sought-after goal. In this framework, cellulose nanocrystal (CNC) has recently emerged as an appealing natural biopolymeric scaffold easily accessible from various renewable sources on industrial scale [1]. It has been recently investigated for the preparation of advanced nanomaterials in many applicative areas [1]. Of note, its stiff chain architecture makes CNC an excellent platform for the fabrication of metal nanohybrids [1]. In this communication, we describe the recent contribution of our research group in the field [2]. In particular, we have recently described an eco-friendly protocol that allows accessing to a hybrid cellulose-based glyconanomaterial. Owing to its unique structure, the post-functionalization of our glyconanomaterial with one or two different headgroups is easily undertaken, by exploiting a robust protocol, under strictly controlled reaction conditions. As detailed in our communication, our approach provides a versatile platform with biomolecular recognition properties (**Figure 1**).

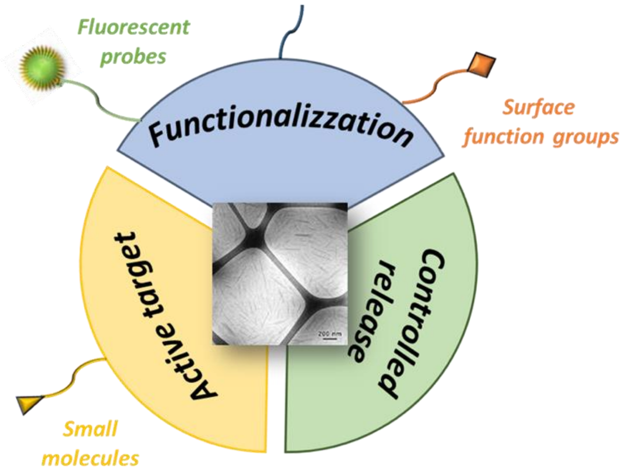

Figure1

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Funder: Project funded under the National Recovery and Resilience Plan (NRRP), Mission 4 Component 2 Investment 1.4 - Call for tender No. 3277 of 30 December 2021 of Italian Ministry of University and Research funded by the European Union – NextGenerationEU; Award Number: Project code ECS_00000017, Concession Decree No. 1055 of 23 June 2022 adopted by the Italian Ministry of University and Research, CUP B83C22003930001, project title “Tuscany Health Ecosystem – THE”.

POS14

Synthesis and characterization of β-myrcene/styrene copolymer

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In recent years, there has been an increasing effort to move away from fossil sources as raw materials for monomer production. Terpenes can be used as raw materials for synthesizing new classes of polymers to make the best use of available biodiversity and to follow the principles of green chemistry.

A new class of materials that reflects these criteria is represented by myrcene-styrene copolymers. These copolymers are known for their unique and versatile properties. Myrcene, an olefinic monomer obtained from biomass, is combined with styrene, an aromatic monomer, to produce copolymers with a wide range of adjustable properties, depending on the composition and polymerization conditions.

Styrene-myrcene copolymers combine the flexibility, impact resistance, and good compatibility of myrcene-based polymers with the rigidity, thermal resistance, and transparency of polystyrene.

The copolymerization was conducted using a titanium complex as catalyst activated with MAO. Polymerizations were carried out at 70°C under nitrogen atmosphere [1].

Samples with myrcene/styrene ratios 30/70, 50/50, 70/30 and 80/20 mol/mol were synthesized and characterized. The glass transition temperature (T_g) increases with increasing styrene content. Differential scanning calorimetry thermograms show relaxation phenomena close T_g, attributed to styrene sequences, as highlighted by annealing experiments at different temperatures. All samples are amorphous. They show X-ray powder diffraction profiles characterized by a double halo typical of polystyrene, and remain amorphous even after annealing treatments. Copolymers with styrene content higher than or equal to 30 mol% show a highly rigidity and experience viscous flow upon stretching at 70°C. The sample with 20mol% appears as a soft material, able to flow even at 40 °C, having a high potential to behave as a rubber upon vulcanization.

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POS15

Efficient Nimesulide degradation by hypochlorite and UVA irradiation: kinetics, reactive species generation and transformation mechanism

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The efficient degradation of Nimesulide (NIM), an emerging pollutant [1], was investigated using a combined approach of chlorination and UVA irradiation (UVA/HClO) [2]. This study aimed to elucidate the kinetics, reactive species generation, and transformation mechanism involved in the degradation process. Additionally, the applicability of the process was assessed in spiked real wastewater samples, and the feasibility of using natural sunlight as a light source was evaluated.

The research revealed that NIM exhibited low reactivity towards hypochlorite (OCl-) alone, requiring the use of additional methods to enhance its degradation. UVA irradiation was employed to activate the oxidizing agent, leading to the complete degradation of 25µM of NIM in 180 min.

To evaluate the radical species formed during the process chemical probes experiments and electron paramagnetic resonance (EPR) experiments were conducted. High-performance liquid chromatography-mass spectrometry (HPLC-MS) analysis revealed the presence of new oxidation compounds, previously unreported in the literature. Among these products, different chlorination patterns and modification of functional groups compared to the initial NIM molecule were characterized. The degree of mineralization was assessed using total organic carbon (TOC) analysis, confirming the efficient degradation of NIM during the UVA/HClO process. Furthermore, the applicability of the process was demonstrated in real wastewater samples where 10 µM of NIM was degraded up to 60% after 60 min. Moreover, the feasibility of utilizing natural sunlight as an alternative light source for the process was proven.

The results contribute to a better understanding of the kinetics, reactive species generation, transformation mechanism, and real-world applicability of the efficient degradation process. This research opens possibilities for the development of sustainable strategies based on the solar light activation of HClO synergistic effect for the removal of NIM and other emerging pollutants in wastewater treatment processes.

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POS16

"Chemical and δ^{13}C isotopic characterization of Aceto Balsamico Tradizionale di Modena PDO aroma compounds by HS-SPME-GC/FID and GC-IRMS techniques: a multivariate approach "

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The Aceto Balsamico Tradizionale di Modena PDO, ABTM, is undoubtedly one of the most peculiar denomination foods among the typical Italian products. Among its various distinctive features, its production process makes it truly unique worldwide. The particular raw material, extended aging period within batteries of different wooden barrels combined with the yearly topping-up procedure all play a crucial role in shaping its sensory and gustatory attributes: a dense and viscous product, dark brown in color, simultaneously sweet and sour and the typical balsamic aroma are the distinctive features of this food. One of the most crucial aspects of managing vinegar cellars is certainly understanding the processes occurring within the battery, inside each barrel, which determine the transformation of the raw material into the final product. To further characterize the uniqueness and peculiarities of the product, some producers have chosen to start batteries with casks of a single essence in order to further underline aromas and flavors of the ABTM. The slow production process induces transformations within the product, amplifying certain compositional differences characteristic of the equilibrium between the liquid and gaseous phases inside each barrel, and magnifying the phenomena of mass-dependent isotopic fractionation of some peculiar ABTM compounds, such as acetic acid. The goal was to identify and differentiate the aromatic profiles of ABTM under various aging conditions. Through GC/MS, over 30 compounds contributing to the aroma of ABTM were identified. These compounds include esters, aldehydes, alcohols, and other volatile organic compounds, which play a significant role in shaping the sensory attributes of the vinegar. By combining the data from HS-SPME-GC/FID analysis with multivariate statistical techniques such as Principal Components Analysis, PCA, significant differences were observed between ABTM and vinegars with a lower degree of aging. Gas Chromatographic Isotopic Ratio Mass Spectrometry, GC-IRMS, technique was used to evaluate the isotopic ratio changes of carbon in specific compounds within the volatile fraction, with the aim of characterizing the ABTM production process and its evolution over time. These findings contribute to a better understanding of ABTM sensory attributes, production techniques, and quality assessment, thus ensuring the continued excellence of this renowned culinary treasure.

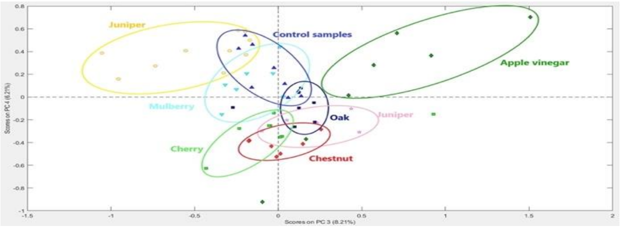

Figure 1: PCA analysis of GC/FID chromatograms of ABTM from batteries with casks made with different woods.

POS17

Molecular tailoring of acceptor and donor moieties for red thermally activated delayed fluorescence emitters for coreactant electrochemiluminescence applications

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Electrochemiluminescence (ECL) can be considered one of the most powerful analytical techniques. It is characterized by (electro)chemical generation of excited species, so since excitons are produced through a non-radiative process, singlet and triplet excited states are populated statistically in a 1:3 ratio. Phosphorescent transition metal complexes represent a good class of emitters thanks to the strong spin-orbit coupling due to the presence of a heavy atom, that favors the intersystem crossing allowing both singlet and triplet excited states to contribute to the emission [1].

Recently, a new strategy to harvest triplet excitons was reported, namely Thermally Activated Delayed Fluorescence (TADF) [2], which can be observed in organic molecules based on a tilted donor-acceptor (D-A) structure. From the tilted structure follows that HOMO and LUMO result spatially separated and that singlet and triplet excited states are divided by a small energy gap (ΔE_{ST}). The small energy gap favors a reverse intersystem crossing (RISC) process that can be promoted by thermal energy and can lead to internal quantum efficiency up to 100%.

Starting from a previous work [3], diphenylamine and tertbutyl carbazole have been chosen as donor moieties, while terephthalonitrile and dipyridophenazine have been tested as acceptors to obtain red emitting TADF dyes.

Cyclic voltammetries, photoluminescence quantum yields and excited state lifetimes of the compounds in solution were recorded. The compounds displayed suitable reduction potentials to be tested as dyes in ECL using TPrA as co-reactant. Assuming $Ru(bpy)_3(PF_6)_2$ as standard, the ECL efficiencies of the compounds were determined and correlated with the electrochemical and photophysical properties of the dyes. Interestingly, 4DPATPN, was found to be the best performing luminophore, with an ECL efficiency almost two times the one of the standard.

Acknowledgements

The authors are grateful to the financial support from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (grant agreement no. 949087).

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POS18

Pyrrolobenzoxazepines (PBOXs) and pyrrolonapthoxazepines (PNOXs) analogs: a novel series of potentially proapoptotic and autophagy modulators

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Apoptosis and autophagy are both physiological mechanisms aimed to preserve the homeostasis in the organism. In the last decade pyrrolobenzoxazepines (PBOXs) and pyrrolonapthoxazepines (PNOXs), a subgroup of microtubule targeting agents (MTAs), have been developed as potential anticancer agents [1][2]. Both PBOXs and PNOXs have shown a significant antiproliferative activity against an extensive range of cancer forms. These compounds exert their microtubule-destabilizing activity through the binding with tubulin [3]. Taking into account the intriguing biological activity shown by these lead compounds, we have developed a new set of compounds having an appropriately functionalized oxazepine core. In addition, we focused on the synthesis of new derivatives introducing a new moiety fused with the oxazepine-core system, which characterizes all the PBOXs and PNOXs. The new moiety could lead to new interactions in the binding site improving the pharmacokinetic profile and the biological activity.

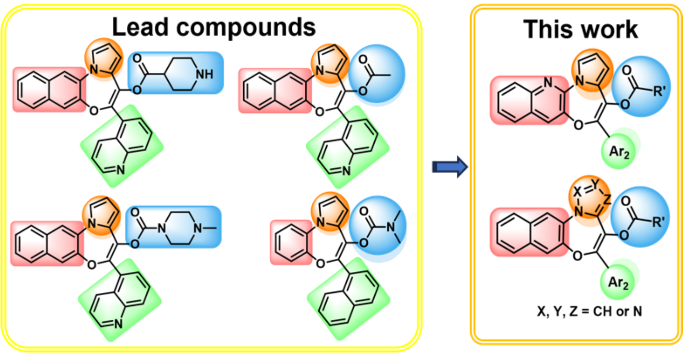

Figure 1: Development of novel PBOXs and PNOXs analogues.

[1] G. Campiani, T. Khan, C. Ulivieri, L. Staiano, C. Papulino, S. Magnano, S. Nathwani, A. Ramunno, D. Lucena-Agell, N. Relitti, S. Federico, L. Pozzetti, G. Carullo, A. Casagni, S. Brogi, F. Vanni, P. Galatello, M. Ghanim, N. McCabe, S. Lamponi, M. Valoti, O. Ibrahim, J. O'Sullivan, R. Turkington, V. P. Kelly, R. VanWemmel, J. F. Díaz, S. Gemma, D. Zisterer, L. Altucci, A. De Matteis, S. Butini, and R. Benedetti, *Eur. J. Med. Chem.* 235 (2022) 114274

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[3] M. Brindisi, C. Ulivieri, G. Alfano, S. Gemma, F. de Asís Balaguer, T. Khan, A. Grillo, G. Chemi, G. Menchon, A. E. Prota, N. Olieric, D. Lucena-Agell, I. Barasoain, J. F. Diaz, A. Nebbioso, M. Conte, L. Lopresti, S. Magnano, R. Amet, P. Kinsella, D. M. Zisterer, O. Ibrahim, J. O'Sullivan, L. Morbidelli, R. Spaccapelo, C. Baldari, S. Butini, E. Novellino, G. Campiani, L. Altucci, M. O. Steinmetz, and S. Brogi, *Eur. J. Med. Chem.* 162 (2019) 290-320

POS19

Development of new and selective peptide targeting FSH receptor for high malignant cancer

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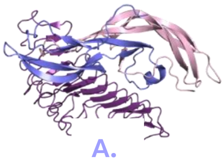
Follicle-stimulating hormone (FSH) is a heterodimeric glycoprotein consisting of two subunits: α and β [1]. The first subunit is common to several hormone meanwhile β subunit provides functional specificity and ensures a specific interaction with FSH receptor (FSHR). Recently has been demonstrated that is overexpressed by a wide range of human and murine cancer cells, human patient-derived tumor xenografts of triple-negative breast cancer and patient-derived cancer tissues. Consequently, for these tumors FSHR may represent an alternative target for diagnosis and treatment [2].

To this aim, the most successful peptide selected due to its antagonistic activity has been proven to be the linear peptide FSH$_{\beta33\text{-}53}$. FSH$_{\beta33\text{-}53}$ has been investigated by Santa Coloma et al. [3] for ovarian cancer targeting, aiming to the design and development of different FSHR-specific (radio)drugs for cancer imaging and therapy.

Starting from x-ray structural studies of the receptor, FSH$_{\beta42\text{-}50}$ peptide sequence, included in FSH$_{\beta33\text{-}53}$, has been synthetized, whose residues are directly involved in the interaction with the receptor. This sequence has been chosen to validate new FSHR-specific peptide probes for the creation of future radiopharmaceuticals directed against FSHR-expressing tumors and tumor blood vessels. To achieve this, the fluorescent probe Cy5.5 has been selected and the synthesis of FSH$_{\beta42\text{-}50}$-Cy5.5, together with FSH$_{\beta33\text{-}53}$-Cy5.5 and their scramble peptides have been performed and the interaction of peptides with FSHR has been evaluated.



A.

FSH$_{\beta42\text{-}50}$

Ac-K(Cy5.5)P^{42}ARPKIQKT^{50}-NH$_2$

FSH$_{\beta33\text{-}53}$

Ac-K(Cy5.5)Y^{33}TRDLVYKDPARPKIQKTCTF^{53}-NH$_2$

B.

Figure 1 – (A.) Crystal structure of human FSH, with FSHα and FSHβ subunit, complexed with its receptor[1](B.) Schematic representation of FSH$_{\beta33\text{-}53}$-Cy5.5 and FSH$_{\beta42\text{-}50}$-Cy5.5.

[1] Fan & Hendrickson **2005**. *Nature*, 433(7023), 269-277.
[2] Wang et al. **2021**. *Animals*, 11(4), 1134.
[3] Santa Coloma et al. **1990**. *Biochemistry*, 29(5), 1194-1200.

POS20

Facile synthesis of 2D MoS_2/BiOI heterojunctions as photoanodes

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BiOX (X=Cl, Br, I) are gathering significant attention as photoelectrocatalysts due to their specific photoelectric properties. Among these compounds, BiOI has aroused the main interest due to its narrowest band gap [1], [2]. Moreover, with a layered tetragonal crystal structure, BiOI is possible to be exfoliated and made into 2D layered form and the band gap can be enlarged during the process meanwhile. However, pure BiOI can suffer from fast charge recombination during the photoelectrocatalytic (PEC) reactions. Therefore, a strategy of inhibiting the charge recombination is required to improve the PEC properties, for example creating heterojunctions. MoS_2 is a popular 2D layered material and has been used in various types of heterojunctions as an efficient co-catalyst for charge separation and transfer. There are two different phases of 2D MoS_2, namely the semiconductive 2H phase and metallic 1T phase, and both of them have the potential to modify the PEC properties of BiOI. Moreover, the 2D structure of both materials provides a high possibility of fabricating van der Waals heterojunctions (vdW HJs) between the interfaces. In this work we report a simple liquid-phase exfoliation method to obtain the MoS_2/BiOI vdW HJs with 2H and 1T MoS_2, respectively. These materials are applied as photoanodes under different light sources to test the intensity of the photocurrent. Interestingly, we found that the photoresponse of the two HJs varies depending on the wavelength of the light source, and further mechanism behind the phenomenon needs to be investigated.

[1] J. Xiong, X. Zhu, J. Xia, and J. Di, Applied Surface Science 627 (2023) 157338
[2] K. M. Alam, P. Kumar, P. Kar, U. K. Thakur, S. Zeng, K. Cui, and K. Shankar, *Nanoscale Adv.* 1 (2019) 1460-1471

POS21

Carboxymethylcellulose amidation under very mild reaction conditions using DMTMM as a condensing agent

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Cellulose is the most abundant biopolymer on Earth. It is mainly obtained from wood through chemical-physical processes, but important quantities can also be obtained from waste biomass[1]. The possibility to use a biodegradable and biocompatible material as a candidate to replace petroleum-derived materials has prompted the scientific community to explore the possible modification of this biopolymer to give it specific properties to be exploited in various applications[2]. In this work the preliminary studies for the chemical modification of carboxymethylcellulose (sodium salt) (CMC) have been reported (Fig. 1). The reaction was carried out in water at room temperature for 20 h in the presence of 4-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-methyl-morpholinium chloride (DMTMM) as condensing agent in analogy to what reported in the literature[3]. The by-products are water soluble and therefore easily removed by dialysis. From the first characterizations (^1H NMR) it emerged that 30% of the carboxyl groups were converted. This synthetic strategy could constitute a way to produce hydrophobic CMC films.

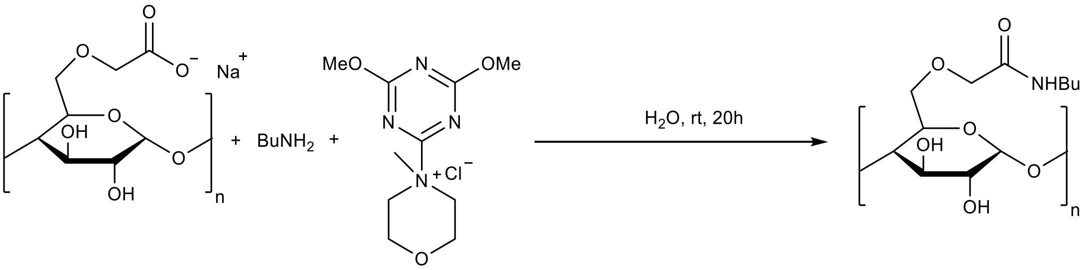

Figure 1: amidation of CMC sodium salt

[1] Heinze T., El Seoud O. A., Koschella A., *Cellulose derivatives: synthesis, structure, and properties* (Springer), 2018.

[2] Tariq A., Farid A., Haq F., Kiran M., Ullah A., Zhang K., Li C., Ghazanfar S., Sun H., Ullah R., Ali A., Muzammal M., Shah M., Akhtar N., Selim S., Hagagy N., Samy M., Al Jaouni S., *Polymers* (2022) 3206-3240.

[3] Sole R.,Gatto V.,Conca S., Bardella N., Morandini A., Beghetto V., *Molecules* (2021) 191-205.

POS22

Hydroformylation of unsaturated organic molecules

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Hydroformylation, also known as the oxo process, involves the metal-catalyzed addition of syngas (CO and H_2) to olefins to form homologous aldehydes. Since its discovery in the early 1900s, it has emerged as one of the largest homogeneously catalyzed reactions in the industry. Nearly all transition metals of the groups 6 to 10 show catalytic activity for hydroformylation, although cobalt and rhodium derived catalysts are the most active. Specifically, the latter is by far the most widely used, showing a 10^4 times faster rate than comparable cobalt catalysts. Despite its importance and versatility, hydroformylation often suffers from the issue of controlling chemo-, regio-, and stereoselectivity. The reaction leads, unless symmetric substrates are used, to a mixture of regioisomeric products, linear and branched. Typical side reactions of the hydroformylation reaction are hydrogenation and alkene isomerization. The latter may even be desirable as in the case of the isomerizing hydroformylation of internal alkenes to n-aldehydes. The aim of this project, that has been developed in collaboration with Polynt S.p.A., is to optimize the hydroformylation of substrates derived from the value chain of the company.

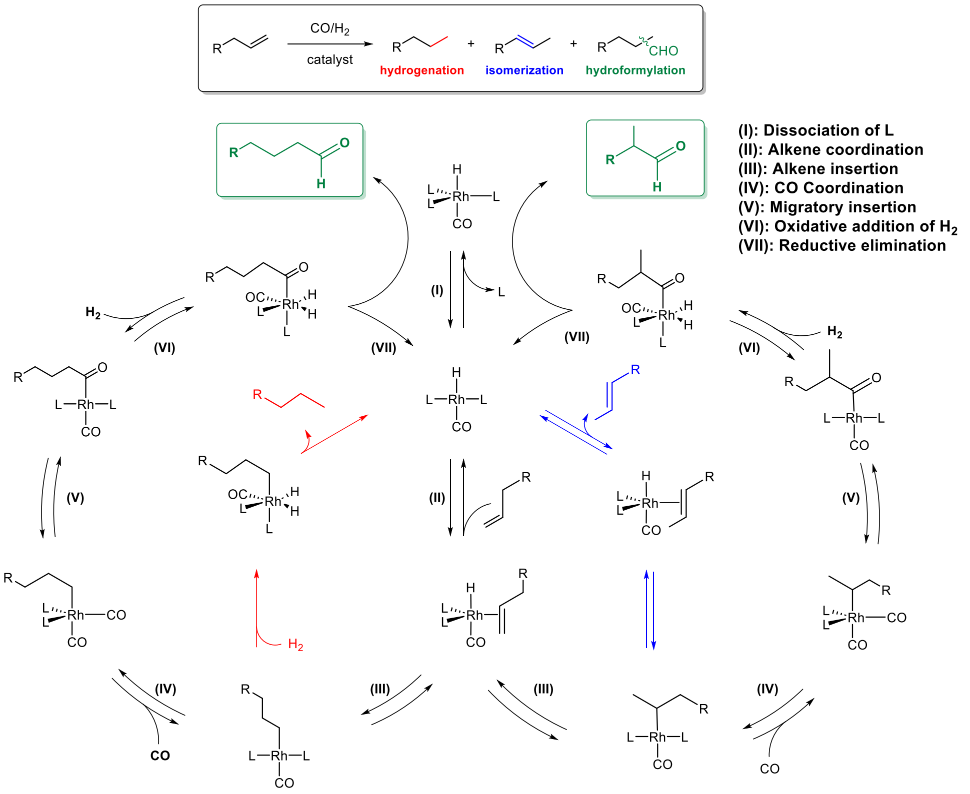

Figure 1: Side reactions and mechanism in the hydroformylation reaction.

POS23

Synthesis of conjugated aromatic polymers as electrodes for secondary batteries with tailorable redox pendants

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Nowadays our everyday life is strongly intertwined to the use of portable electronic devices, such as phones, laptops, smartwatches, and Bluetooth headsets. Year by year, the demand for systems capable of efficiently and reliably storing high amounts of energy is increasing. The aim of this project is to prepare new, high-performance polymeric materials that can be employed as electrodes.

The use of materials of organic nature offers significant advantages such as high specific capacity (due to their intrinsic low density), the possibility of modulating their properties during the synthetic steps according to the application needs, milder synthesis conditions, and greater sustainability (both due to the absence of cobalt and ease of recycling or disposal). However, organic electrodes are also characterized by important limitations that impede their technological growth, such as low performance, limited conductivity, and rapid performance deterioration.

In the course of this study, in order to overcome these problems, we developed non-conjugated polymer precursors, characterized by high molecular weight and good processability, which can be transformed into electroactive conjugated polymers through a final reaction with high yield and selectivity, that can could find application as versatile material for electrodes in secondary batteries.

In particular, these precursor polymers comprise aromatic or heteroaromatic units-such as anthraquinone, fluorenone, or thiophene which are connected via 1,4-diketonic bridges. The introduction of these latter between the various aromatic rings increases the flexibility of the macromolecular chains and allows an easy functionalization with a primary amine through the Paal-Knorr reaction.

Such reaction yields a N-substituted pyrrole ring and thus fully conjugated polymers can be obtained. This strategy can be used to insert various active redox groups, responsible for the charge and discharge cycles, as pendants to the conjugated main chai. Compared to non-conjugated redox polymers, this increases the overall conductivity of the system, therefore overcoming the kinetic limitations related to their insulating nature. Moreover, the synthetic process allows the insertion on multiple redox centers, making this materials appealing also for the application as chemoresistive probes and active materials in organic electrochemical transistors (OECTs).

POS24

Zinc Imidazolate Framework-8 (ZIF-8) for biomedical applications

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Zeolitic Imidazolate Framework, in particular *sod*-Zn(mIM)$_2$, also known as ZIF-8 is a subclass of MOF formed by the self-assembly of zinc ions and 2-methylimidazole. ZIF-8 has attracted considerable attention due to its high thermal and moisture stability compared to other MOF structures. It shows excellent biocompatibility, stability under physiological conditions and responsiveness to the weak acidic environment associated with malignant tumors and other diseases [1].

As illustrated in *Figure 1*, in this work its use is investigated in three different applications: *a)* encapsulation of snail slime extracted from *Helix aspersa muller* [2]; *b)* Cellulose/ZIF-8 hybrid paper for antibacterial patches; *c)* modification of titanium scaffolds.

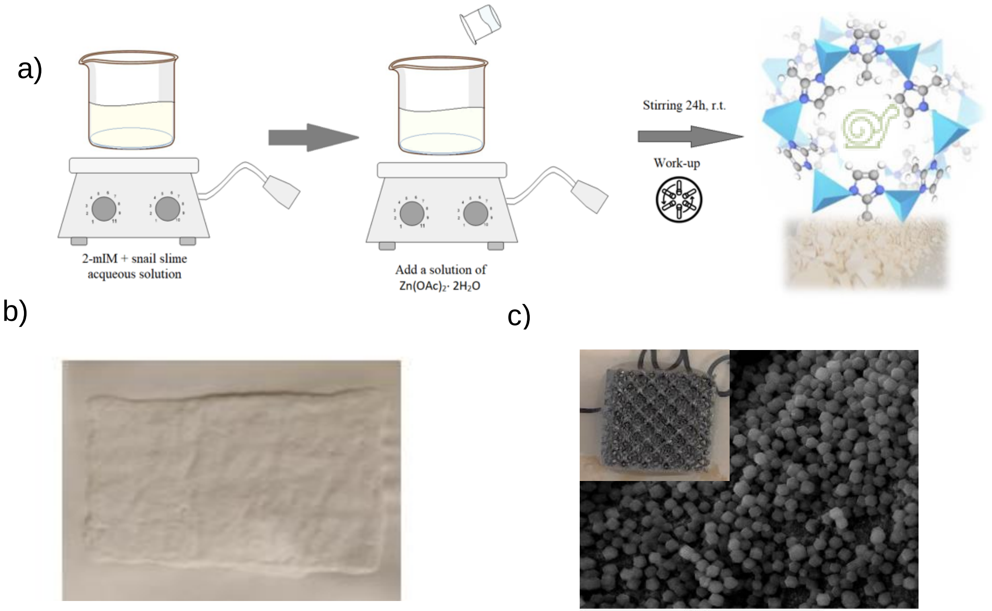

Figure 1: Scheme of the encapsulation of slime in the ZIF-8 (a), Cellulose/ZIF-8 hybrid paper (b) and a sample of ZIF-8 on titanium scaffold (c).

[1] Hoop, M. *et al.*, *Appl. Mater. Today* **2018**, *11*, 13.

[2] Di Filippo, M.F.; Di Matteo, V.; Dolci, L.S.; Albertini, B.; Ballarin, B.; Cassani, M.C.; Passerini, N.; Gentilomi, G.A.; Bonvicini, F.; Panzavolta, S., *Nanomaterials* **2022**, *12*, 3447.

POS25

Enhancing Ce6 performances in PDT by conjugation with a Fullerene-C_{60}

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Chlorin e6 (Ce6) is one of the most widely used photosensitizers, due to its high efficacy in singlet oxygen generation, low dark toxicity and great absorption in the red region of the visible spectrum (650-700 nm) [1]. However, the negative charges of the carboxylic groups of Ce6 limit its performances as photosensitizer, resulting in a poor ability to permeate the cellular membrane.

Fullerenes are nanomolecular carbon cages commonly used as platforms for the delivery of drugs and imaging agents, because of their ability to pass through cell membranes to deliver therapeutic molecules [2].

Here we synthesized and fully characterized a covalent Chlorin e6 - Fullerene dyad (C_{60}-Ce6) (figure 1).

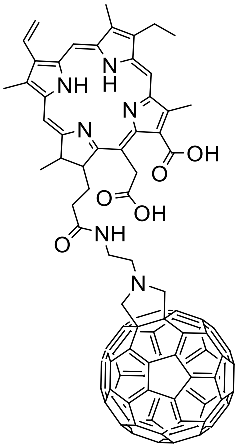

Figure 4. *Chemical structure of the C_{60}-Ce6 Dyad*

Upon irradiation with red light, C_{60}-Ce6 showed a large production of ROS via both type I (peroxides) and type II (singlet oxygen) mechanisms. In particular, the type I pathway was largely enhanced compared with free Ce6, suggesting the formation of an interacting antenna-fullerene system [3].

In vitro tests demonstrated the increase of the cellular uptake of the C_{60}-Ce6 molecule compared to free Ce6, along with an enhancement of the killing efficacy of the dyad, upon irradiation with red light.

[1] A. Hak, M. S. Ali, S. A. Sankaranarayanan, V. R. Shinde, and A. K. Rengan, *ACS Appl. Bio Mater.*, 6 (2023), 349-364
[2] A. Montellano, T. Da Ros, A. Bianco, and M. Prato, *Nanoscale,* 3 (2011), 4035-4041
[3] Q. Li, C. Huang, L. Liu, R. Hu, and J. Qu, *Cytometry Part A*, 93A (2018), 997-1003

POS26

Design of innovative high-performance polymers for passive lunar dust mitigation

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The Moon is covered by a thin layer of dust, composed of a granular material of various shapes and sizes, and comprised of a diverse collection of mineralogical compositions [1]. These particulates are porous abrasive, chemically reactive, electrostatically charged, and sometimes magnetic and adhere strongly to exposed surfaces Therefore, lunar dust is now recognized as a major concern for lunar surface missions.

The design and development of innovative high performance, lightweight polymers exhibiting superior passive dust mitigation capabilities against lunar regolith micrometric dust particles is of great interest for the future space missions. Aromatic polyimides are promising materials thanks to high thermal stability and hydrophobic properties. A designed novel molecular structure of polyimides and a suitable modification of their surface chemistry allow improvement the property to mitigate lunar dust adhesion. This has been achieved by introducing within the polyimide matrix special low molecular weight additives, able to spontaneously migrate toward the polymer's surface by favorable thermodynamic interactions at the polymer-air interface. This approach allows enabling the controlled chemical modification of the material surface, in order to minimize the electrostatic and the van der Waals interactions among the external layers and the granular particles, and keeping the inherent properties of polyimides, including the high thermal stability, mechanical strength, and radiation resistance.

Low surface energy aromatic copolyimides have been synthesized and characterized. The materials have exhibited very interesting optical properties (Figure 1), excellent thermomechanical properties suitable to withstand the extreme space environment conditions, and superhydrophobic properties suitable to mitigate adhesion of dust particles of lunar regolith.

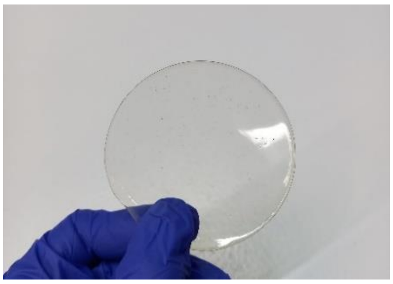

Figure 1: Transparent film of synthesized polyimide

[1] L.A. Taylor, T. T Meek, *J. Aerospace Eng*.Vol.18 (2005), 188.

POS27

Development of sustainable food packaging through the integration of the polyolefin crosslinking control technique in multilayer film technology

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Food packaging is the main cause for the huge volumes of plastic waste that often cannot be recycled and that are destined for landfills or released into the environment [1]. The development of sophisticated technologies, such as the production of multilayer films by co-extrusion of different polymers, has allowed the design of technical films for food packaging with specific properties for each food able to perform different functions, such as food protection, as required by food safety and increasing their shelf life. However, this development has reduced the possibilities of mechanical and chemical recycling of plastic waste deriving from food packaging because the technical films are made up of layers of different polymers that are difficult to separate [2]. Due to the difficulties in separating different polyolefins and the chemical incompatibility between different polyolefins, in particular between polyethylene (PE) and polypropylene (iPP), the products deriving from recycling mixtures of PE and iPP show worse properties than those of the original components [3].

To improve the properties of products deriving from the secondary recycling of plastic waste, and consequently increase the recycling percentages, a strategy has been developed which involves the introduction of a certain degree of crosslinking with the formation of chemical bonds between the macromolecules which allows to reduce the thickness of the polymeric films without modifying their barrier and food protection properties. On the one hand, this strategy significantly reduces the volume of plastic waste derived from food packaging and, on the other hand, significantly increases the chances of mechanical recycling of the films themselves, without causing downcycling.

A study of the strategies to produce polymeric films that integrates the controlled crosslinking technique of polyolefins in the industrial technology of multilayer film production by coextrusion is presented. This technology not only improve the properties of the films by reducing their thickness but also, improve the possibility of recycling and environmental sustainability of the packaging. Specifically, the optimal degree of crosslinking and of the minimum thickness of the various layers will be evaluated from the analysis of the physical and mechanical properties of crosslinked multilayer films and fine-tuning of the industrial production of recyclable multilayer films that can replace the current products used for food packaging, after passing the recyclability tests.

[1] Plastics – the Facts 2019. "An analysis of European plastics production, demand and waste data". Plastics Europe, 2019

[2] Schyns, Z. O. G., Shaver, M. P. "Mechanical Recycling of Packaging Plastics: A Review". Macromol. Rapid Commun. 2020, 2000415

[3] Graziano, A., Jaffer, S., Sain, M., "Review on modification strategies of polyethylene/polypropylene immiscible thermoplastic polymer blends for enhancing their mechanical behavior". J. Elastomers Plast. 2019, 51, 291−336

POS28

Opportunities for new orthosteric/allosteric ligands of cannabinoid receptors

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Cannabinoid receptors (CBRs, CB1R and CB2R) are crucial in various biological processes and physiological functions. Since their discovery, many efforts have been made to develop highly selective orthosteric CBR ligands for therapeutic purposes. However, direct-acting agonists often cause adverse effects, limiting their clinical development. Recent cannabinoid research has explored bitopic modulation as a potential therapeutic approach to avoid the side effects of orthosteric ligands [1][2]. By simultaneously interacting with orthosteric and allosteric binding sites on the same receptor, a bitopic ligand can improve binding affinity, subtype selectivity, and activate specific pathways while sparing those that mediate unwanted effects, resulting in improved therapeutic profiles. The current project proposes the design, synthesis, and biological evaluation of RF compounds (Figure 1) as new orthosteric/allosteric ligands of CBRs. These compounds consist of two distinct pharmacophoric units, a CB1R ago-PAM and a CBR orthosteric agonist, bridged through a variable-length linker. The newly developed compounds were extensively tested in binding and functional assays. Furthermore, computational studies have enabled us to gain new insights into dual orthosteric/allosteric stimulation of CBRs.

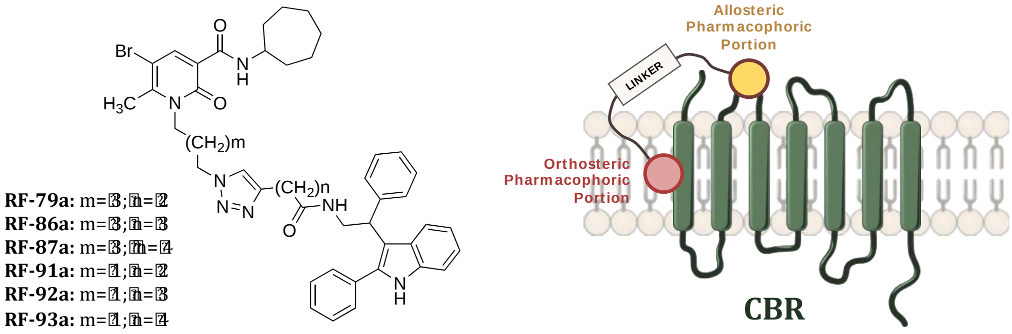

Figure 1: General structure of RF ligands.

[1] F. Gado, R. Ferrisi, B. Polini, K.A. Mohamed, C. Ricardi, E. Lucarini, S. Carpi, F. Domenichini, L.A. Stevenson, S. Rapposelli, G. Saccomanni, P. Nieri, G. Ortore, R.G. Pertwee, C. Ghelardini, L. Di Cesare Mannelli, G. Chiellini, R.B. Laprairie, and C. Manera. *J Med Chem* 65,14 (2022) 9918-9938.
[2] R. Ferrisi, B. Polini, C. Ricardi, F. Gado, K.A. Mohamed, G. Baron, S. Faiella, G. Poli, S. Rapposelli, G. Saccomanni, G. Aldini, G. Chiellini, R.B. Laprairie, C. Manera, and G. Ortore. *Int J Mol Sci* 24, 3 (2023) 2135.

POS29

Synthesis and assembly of responsive amphiphiles for targeted diagnostics and drug delivery

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Over the last couple of decades, functional supramolecular systems have played an important role in the design of innovative materials leading to a remarkable variety of applications in therapeutics, such as drug delivery. It is known that drug delivery systems face several obstacles regarding the distribution, targeting efficiency and the specificity of drug release. In biomedical applications, polyethylene glycol (PEG) functionalization has been an important approach for modifying nanocarriers, such as lipid-based vesicles (liposomes), to avoid phagocyte-mediated uptake and to prolong their circulation time in the blood. However, this approach faces limitations with regards to cell-targeting [1].

The current project aims to develop stimuli-responsive nanosystems that possess crucial stealth properties, but which could switch on their cell-targeting properties only in the presence of the desired stimuli, such as light. More specifically, this study explores the assembly of PEGylated lipids with conventional phospholipids (e.g., POPC) and targeting ligands to develop stealth liposomes. Coumarin derivatives behave as linkers that join together the PEG chain with the hydrophobic tail of the lipid via a carbonate bond that can be irreversibly cleaved, leading to the elimination of the PEG-coumarin system, and allowing the tumor-targeting ligands on the liposome to be exposed (Figure 1). Previous work in our group has studied the self-assembly of stimuli-responsive amphiphiles to form nanovesicles and giant unilamellar vesicles [1, 2]. Our aim is to explore this approach for diagnostic applications and targeted delivery of therapeutics, as well as in vesicle-vesicle systems communication.

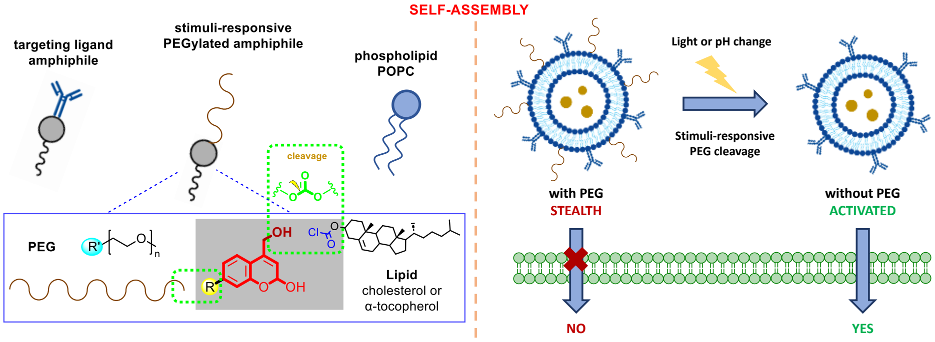

Figure 1: Self-assembly of amphiphiles for the formation of stimuli-responsive stealth liposomes.

[1] Q. He, J. Chen, J. Yan, S. Ci, H. Xiong, Y. Liu, D. Peng, M. Mo and Z. Liu, *AJPS* 15 (2020), 416–448
[2] C. Z. J. Ren, P. Solís Muñana, J. Dupont, S. S. Zhou and J. L. Y. Chen, *Angew. Chem. Int. Ed.* 58 (2019) 15254–15258
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POS30

Phosphorescent Ir(III)-based metallapolymers: design, synthesis and applicative perspectives

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Phosphorescent metallapolymers have recently gained great interest due to the possibility of endowing polymer materials with bright and often color tunable emission typical of Ir(III) cyclometalated complexes with general formula $[Ir(C\^N)_2(N\^N)]^{0/+}$ [1]. In this context, we designed a series of "polymerizable ligands" capable of coordinating the metal center and, at the same time, being able to copolymerize with methacrylic monomers. To this end, we equipped three well-known diimine ligands (N^N) [2,3] with a polymerizable styryl unit. Then, metallapolymers were obtained following two complementary pathways involving either the complexation of the pre-formed MMA-L copolymer with different Ir fragments or the direct copolymerization of the mononuclear complexes with MMA. The resulting hybrid materials displayed intense phosphorescence in the solid state, with emission colors spanning from blue to orange depending on the nature of the Ir-based unit. These promising results pave the way for the application of this new class of metallapolymers as Luminescent Solar Concentrators for the photovoltaic technology and/or to solid state lighting.

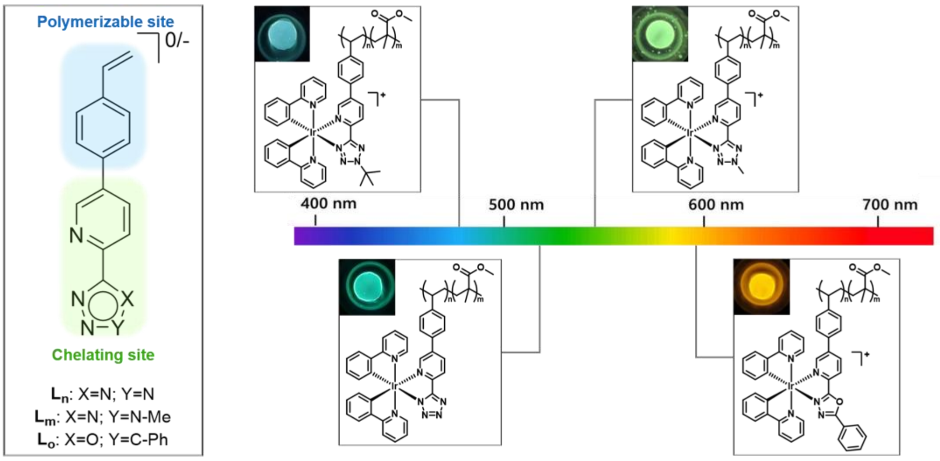

Figure 1: Polymerizable ligands (left) and corresponding metallapolymers (right).

[1] C.L. Ho, W.Y. Wong, *Coordination Chemistry Reviews*, 255 (2011) 2469–2502.
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POS31

Dopamine effect on flexible starch-based films for food packaging applications

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Food packaging plays a crucial role in preserving food quality and extending its shelf life. However, the widespread use of petroleum-derived packaging materials has led to serious environmental concerns [1]. In recent years, the quest for sustainable and biodegradable alternatives has intensified, with flexible starch-based films emerging as a promising eco-friendly option. These biopolymer films possess inherent biodegradability, renewability, and compatibility with various food products, making them highly attractive for food packaging applications. In particular, among these materials, UV-shielding starch films have shown promise due to their ability to provide protection against harmful ultraviolet (UV) radiation, which can lead to food spoilage and degradation of sensitive nutrients.

One of the significant challenges in utilizing starch-based films for food packaging is their hydrophilicity and the limited barrier properties against moisture, oxygen, and other external factors. This limitation can lead to compromised food safety and reduced shelf life. To overcome this hurdle, various techniques have been explored to enhance the performance of starch-based films.

Dopamine is a small amine-rich molecule that in mild alkaline conditions starts the process of oxidative self-polymerization to form polydopamine (PDA) [2]. This, in addition to increasing the hydrophobicity of the materials, has a quinone structure which provides good UV shielding properties.

In this study, the effect of self-polymerized dopamine on flexible starch-based films for food packaging applications will be evaluated.

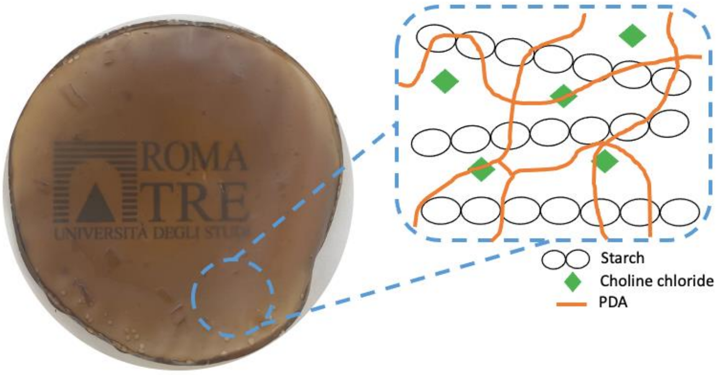

Figure 1. PDA/Starch network

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POS32

Proteomics as a powerful tool to investigate biomarkers in food: authentication of organic chicken meat

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The advent of foodomics technologies is creating new opportunities and challenges food chemistry. Among them, proteomics represents the comprehensive characterization of the expressed proteins in a biological system at a specific given time [1]. Mass spectrometry plays a crucial role in proteomics providing high-throughput technologies that, combined with advanced statistical and bioinformatics tools, can provide a comprehensive view of the proteome and the study of specific biomarkers. The application of proteomics on food matrix from biological complex systems, such as meat and meat products, allows to decipher the underlying cellular mechanisms behind quality and authenticity traits.

Poultry meat is among the most commonly consumed meats in the world. The physiological and metabolic functions of the animals are influenced by many factors such as the production systems and pre-slaughter stress, with consequent impact on the quality of the chicken meat [2]. Organic meat production systems aim to provide more sustainable products with high levels of quality and safety and are based on high animal welfare standards [3]. To date there has been a paucity of published literature on the application of high-throughput omics methods to further our understanding and characterization of these production systems and potential impacts on quality. Thus, the present work has been designed to use for the first time data independent acquisition - mass spectrometry proteomics and chemometrics for the discrimination of two farming systems: organic versus antibiotic-free used to produce chicken meat.

A total of 40 samples including 20 Ross 308 and 20 Ranger Classic chicken early post-mortem breast muscles (10 organics and 10 antibiotic-free for each group) were provided by Fileni® industry (Cingoli, Italy) and served in this trial. The quantitative proteomics was performed applying a shotgun-SWATHMS method using a TripleTOF instrument in Data-Independent Acquisition mode. The applied proteomics allowed the simultaneous identification and quantification of 660 proteins. A clear discrimination between the 4 groups based on their proteome resulted from multivariate statistical analysis. The bioinformatics pathway enrichment analyses, allowed to place the statistically significant abundant proteins, identified as putative biomarkers, in the related metabolic pathways and to understand the complexity behind the impact of animal strains and farming method on meat proteome.

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POS33

Synthesis of a light-responsive PEDOT:PSS bearing azobenzene moieties and its integration in organic electrochemical transistors (OECTs).

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In bioelectronics, organic field-effect transistors (OFETs) and organic electrochemical transistors (OECTs) represent promising bioelectronic platforms allowing a wide range of applications from electrophysiological signals recording to chemical and biological sensing and neuromorphic devices[1]. The large capability of electrolyte ions to penetrate into the organic semiconductor or conducting polymer (CP)-based channel, endow OECTs to operate at low voltages and give OECTs impressive signal amplification properties[2]. Nowadays, an attractive prospect facing OECT lies in the possibility to modulate the output current through an external trigger allowing the development of devices with tailored electrical properties. Among different types of stimuli (T, pH etc.), light is considered the most promising stimulus due to the low invasiveness and the capability to be delivered instantaneously and into a precise location. In this work, a poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) bearing azobenzenes moieties was synthesized through electrodeposition of the precursor N_3-PEDOT:PSS followed by a post-functionalization with alkyne-bearing azobenzenes *via* Huisgen [3+2] azide-alkyne cycloaddition. The so obtained azo-tz-PEDOT:PSS has been fully characterized and integrated as a light-responsive gate eletrode in a OECT architecture. The operation of the azo-tz-PEDOT-based OECT and its output current modulation induced by the presence of the photoswitchable molecules have been demonstrated as well as its application as a neurohybrid building block capable to mimic the retina structure as well as synaptic neural functions such as short- and long-term plasticity.

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POS34

In silico investigation of supramolecular carborane carriers

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The dicarba-closo-dodecaboranes (carboranes) are icosahedral carbon-containing boron clusters. They have the potential to serve as a new type of pharmacophore for drug design and are promising candidates for Boron Neutron Capture Therapy (BNCT) [1]. However, the hydrophobicity of pristine carboranes hinders their direct use in physiological environments. Two different approaches have been used to overcome their lack of solubility: i) synthesis of water-soluble derivatives by chemical functionalization, ii) supramolecular dispersion. Host-guest systems are widely used in medicinal chemistry thanks to their low environmental and economic impact compared to traditional functionalization methods [2].

In this work we use computational techniques to investigate the interactions between pristine carboranes and two different supramolecular hosts: cyclodextrins and cucurbiturils. These macrocycles are commonly used in supramolecular delivery systems and are widely adopted in many pharmaceutical formulations.

The results show that both cyclodextrins and cucurbiturils can bind carboranes in their cavity: i) van der Waal interactions between the guest and the hydrophobic interior of the hosts are the driving force of the binding, ii) the size of the host plays a fundamental role in the encapsulation of the carborane, iii) cucurbiturils displayed a higher affinity than cyclodextrins thanks to their less flexible structure.

This study suggests that cucurbiturils and cyclodextrins represent an effective delivery system for carboranes.

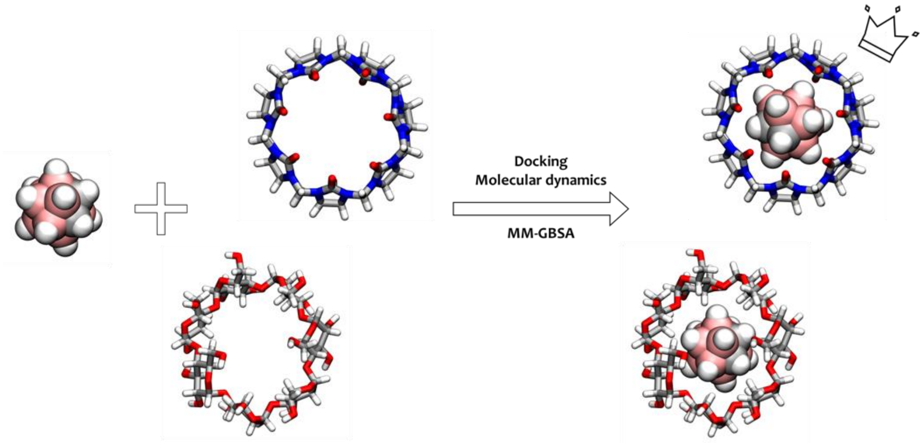

Figure 1: carboranes@hosts inclusion workflow

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POS35

Multipotent Precursors as Immobilization Strategy for Conjugated Polymers with Complementary Electronic Properties

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Indubitably, the development of semiconductors technologies that characterized last century was the turning point that allowed the rise of modern-day electronics and the information revolution we are living. However, despite their success in applications such as OLEDs and flexible electronics, organic semiconductors did not live up to the expectations researchers had 50 years ago. One unrivaled advantage of silicon-based technology over these latter, lies in the possibility of obtaining regions defined by complementary electronic and transport properties - *n* and *p* - on a single substrate, which are at the base of integrated circuits and complementary logic configurations (CMOS). This approach cannot be easily replicated with organic semiconductors due to their intrinsically different nature, which adds up to other shortcomings such as the lower charge mobility and the often non-efficient charge injection from metallic materials.

To avoid these limitations, we are developing a novel approach based on polymeric precursors that allow to prepare high-molecular weight polymers, which are still solution-processable, and are characterized by different electronic properties. During the presentation I will introduce a novel class of polymeric precursors which can undergo two different transformations to yield two different conjugated polymers from the same starting materials. Notably, these materials can be realized so that they show complementary electronic properties, i.e. one comprises high-HOMO units while the other is characterized low-LUMO units. Such transformations are achieved by different chemical treatments, which can also be applied orthogonally and on the solid state, thus generating different phases on a single substrate.

We characterized the systems proposed and show several examples of how this methodology can be applied for the fabrication of OFETs, redox polymers, and multicolored electrochromic displays.

POS36

EC-STM applied to ORR study on M-OEP (M=Zn,Ni,Co)

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The development of new catalysts, that can substitute the expensive Platinum in speeding up the sluggish kinetic of oxygen reduction reaction (ORR), has a crucial importance for the increasing in the production of Proton-exchange membrane fuel cell. MN4 based mesoporous carbon showed promising results as platinum free catalysts [1]. To rationalize the catalytic behavior of MN4-type active sites, macrocyclic MN4 molecular complexes can be used as model catalysts. It is known that a volcano plot correlation arises for different transition metal MN4 chelates with the M(II)/M(III) redox potential or the partial occupation of *d* orbitals of M(II) as reactivity descriptors that, furthermore, correlate with the binding energy of the M-O_2 adduct [2]. Here three type of metal octaethylporphyrins (MOEP), which are in turn ZnOEP, NiOEP and CoOEP, were deposited onto highly oriented pyrolytic graphite (HOPG) substrate and studied with electrochemical scanning tunnelling microscopy (EC-STM) and voltametric techniques. From the voltametric analysis it emerged that CoOEP is the best catalyst for ORR because of the most positive onset potential and highest selectivity with a preference for the 2-electron pathway, on the other hand ZnOEP and NiOEP showed similar results with low activity and 2e/3e mixed selectivity. The EC-STM analysis added new information about the molecular system. It was observed a dip in EC-STM images in the center of molecules both for ZnOEP and NiOEP which remains constant when switching the saturation of the electrolyte from argon to oxygen suggesting no coordination of O_2. On the contrary, CoOEP molecule showed a bright protrusion in the center that halves when switching to oxygen, this effect was already observed in a similar system and associated to O_2 coordination at the CoOEP metallic center [3]. The module of the protrusion is eventually combined with the half peak potential of ORR, extrapolated from voltammograms, to build a reactivity scale of first raw transition MOEP. The resulting graph follows a volcano-like shape where FeOEP occupies the apex and CoOEP places immediately below.

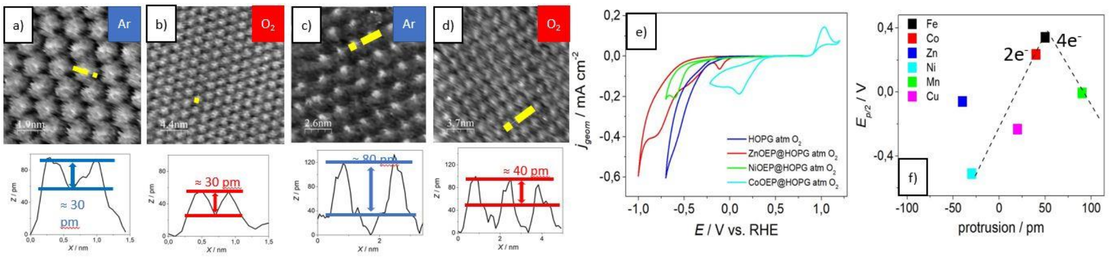

Figure 1: a-d) EC-STM images of a-b) NiOEP, c-d) CoOEP; e) cv of MOEP in O_2 at 50mV/s scan rate; f) volcano-like plot of first raw transition metal OEP.

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POS37

PPARγ non-agonists: a new frontier for a safe anti-diabetic treatment

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Type 2 diabetes mellitus (T2DM) is a major health issue that has reached alarming levels. Today, more than half a billion people are living with diabetes worldwide [1]. Moreover, most of glitazones, the traditional anti-diabetic drugs, which act as Peroxisome proliferator-activated receptor γ (PPARγ) agonist, have been withdrawn from the market. To avoid the serious adverse effects related to the PPARγ agonism profile, a new opportunity is represented by the development of molecules acting as inhibitors of PPARγ phosphorylation by the cyclin-dependent kinase 5 (CDK5). Their mechanism of action is mediated by the stabilization of the PPARγ β-sheet containing Ser245 [2].

Recently, we disclosed the PPARγ non-agonist activity of 4-(4-bromophenyl)-3-hydroxy-5-(3-hydroxyphenyl)furan-2(5H)-one (**1**), which is able to block the phosphorylation of the enzyme without direct inhibition effect of both CDK5 and PPARγ [2]. Crystallographic experiments allowed us to deeply investigate the interaction of **1** with PPARγ, and the co-crystal data (PDB: 8ADF) [2] were used as starting point for the computational studies, leading to optimized derivatives of **1**, endowed with higher affinity for PPARγ.

Of note, an innovative green synthetic approach was tackled in several steps, where the traditional organic solvents were replaced with bio-solvents derived from biowaste, or from very cheap and easily accessible natural sources.

The results of this study will be presented, evidencing that the γ-hydroxy-lactone scaffold may provide a promising template for the development of novel anti-diabetic agents.

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[2] Capelli, D.; Cazzaniga G.; Mori, M.; Laghezza, A.; Loiodice, F.; Quaglia, M.; Negro, E.; Meneghetti, F.; Villa, S.; Roberta Montanari, R. Biological Screening and Crystallographic Studies of Hydroxy γ-Lactone Derivatives to Investigate PPARγ Phosphorylation Inhibition. *Biomolecules* **2023**, 13, 694

POS38

Exploring the molecular mechanisms behind sensitivity in nanoparticle-assisted NMR chemosensing

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Nanoparticle-assisted nuclear magnetic resonance (NMR) chemosensing exploits nanoparticles as supramolecular receptors to detect target molecules in complex mixtures via nuclear Overhauser effect (NOE) experiments, with detection limits down to the micromolar range [1,2]. However, the sensitivity at the basis of such detection limits is little understood. For this reason, NMR spectroscopy and atomistic molecular dynamics simulations has been carried out to examine the molecular interactions behind the sensitivity of different NMR chemosensing experiments (saturation transfer difference (STD), water STD, and high-power water STD, Fig. 1) [3].

Our findings support the fact that the intensity of the observed signals correlates with the number and duration of the spin–spin interactions (between analytes/nanoparticles/solvation molecules). Location and dynamics of each analyte inside the monolayer influence these parameters. These insights will eventually facilitate the tailoring of future experimental and computational setups, making NMR chemosensing an even more effective technique in practical use.

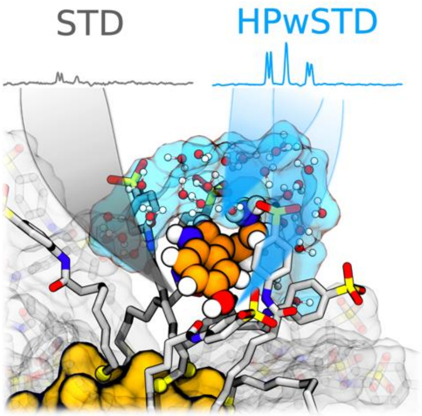

Figure 1: Sensitivity difference between STD and HPwSTD in nanoparticle-assisted NMR chemosensing.

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[2] A. Cesari, D. Rosa-Gastaldo, A. Pedrini, F. Rastrelli, E. Dalcanale, R. Pinalli, and F. Mancin, *Chem. Commun.* 58 (2022) 10861-10864
[3] S.Franco-Ulloa, A. Cesari, L. Riccardi, F. De Biasi, D. Rosa-Gastaldo, F. Mancin, M. De Vivo, and F. Rastrelli, *J. Phys. Chem. Lett.* https://doi.org/10.1021/acs.jpclett.3c01005 (just accepted)

POS39

Solid-phase synthesis of nanoMIPs: how the parameters optimization can improve their binding ability

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The solid phase polymerization synthesis (SPPS) is a versatile and innovative technique to obtain molecular imprinted nanopolymers (nanoMIPs) with very high affinity and selectivity for the target molecules [1]. In this approach, the template molecules are not free in the polymerization medium, but they are immobilized onto the surface of a solid support. The polymerization process takes place in the interstitial space between non-porous glass beads grafted with template molecules. After the polymerization, nanoparticles are obtained with hydrodynamic diameters of 120/150 nm and with imprinted binding sites only on the surface and not in the bulk of the polymeric structure.

This approach presents several practical advantages over the traditional approach: the bleeding effect due to residual template molecules in the imprinted polymer is avoided, grafted templates do not need to be soluble in the polymerization solvent, thus eliminating any issues about solvent-template compatibility. The solid phase can be reused many times, allowing the use of expensive molecules, toxic or harmful templates. Here I present the results of three studies about the optimization of SPPS parameters. In the first study [2], we evaluated the impact, on the binding and the morphological properties of the nanoMIPs, of the use of water and organic environment of synthesis and the use of a spacer arm to graft the template on the solid phase. To perform these studies, we selected a proof-of-concept template: the ciprofloxacin.

In the second study we conducted an experimental design on the formulation of the water-environment synthetized nanoMIPs. We variated the molar ratio of the monomers and evaluated how the binding properties (affinity and selectivity) vary accordingly. We evaluated the variations of these properties through the calculation of the multiple linear regression response surfaces.

Once the best formulation was selected, in the third study [3] we investigated the influence of the polymerization time – ranging from 15 min to 3 hours – on the same properties. Intermediate times (45-60 min) produce nanoMIPs with the highest affinity ($>10^6$ M^{-1}) and good selectivity.

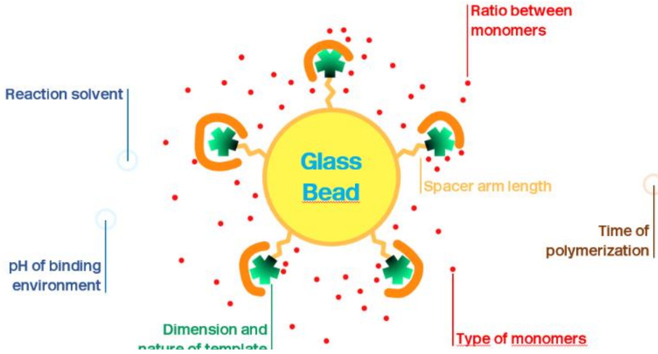

Figure 1: Schematic representation of the synthesis parameters.

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POS40

Highly robust and efficient Blechert-type cyclic(alkyl)(amino)carbene ruthenium complexes for olefin metathesis

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N-Heterocyclic-Carbene (NHC) ruthenium-complexes are recognized for their high catalytic efficiency in Olefin Metathesis (OM), however, they face stability issues in presence of ethylene, a common byproduct for such transformation [1]. Cyclic(alkyl)(amino)carbene (CAAC) ruthenium-complexes do not undergo the common degradation path, being more stable but at the same time less reactive.4 Herein we report on the synthesis and the catalytic activity of a new series of bench-stable CAAC ruthenium-catalysts. The latter, which contains a bulky N-Diisopropyl (DIPP) moiety on the heterocyclic scaffold, capitalizes a strategic Blechert-type activation on the styrene fragment [2]. These new complexes revealed to be highly competent for Ring-Closing Metathesis (RCM), Cross-Metathesis (CM), Ring-Opening Cross Metathesis (ROCM), Macrocyclization at low to very low catalytic loading (10-1000 ppm) and Asymmetric Ring-Opening Cross Metathesis (AROCM) at very low catalyst loading (0.05 mol%). The ethenolysis of Methyl Oleate (MO) has also been accessed by using 5 ppm of catalyst and atmospheric pressure of ethylene instead [3].

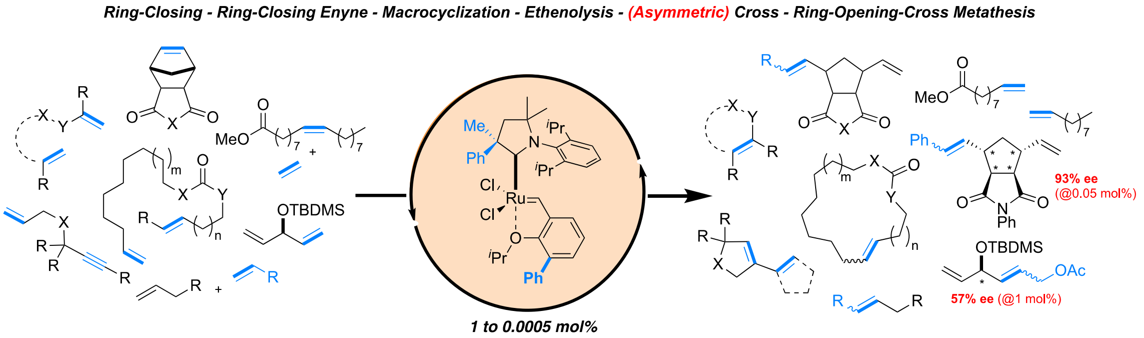

Figure 1: Blechert-type cyclic(alkyl)(amino)carbene ruthenium complexes for olefin metathesis.

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POS41

Mechanistic prediction of the membrane permeability of cyclic peptides through free-energy simulations

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In recent years, cyclic peptides have become an appealing field as due to their size and flexibility enable the binding of macromolecules previously deemed untargetable. However, one of the significant issues hampering their development is the poor permeation of biological membranes, eventually precluding their exploitation for intracellular targets and reducing their oral bioavailability. [1]

Leveraging on publicly available experimental results obtained via PAMPA membrane permeability assay [2], we assembled a dataset including twenty cyclic peptides and peptidomimetics, covering a reasonably wide chemical space and characterized by diverse physicochemical properties.

To understand the molecular basis of the variable passive permeation of cyclic peptides, enhanced sampling algorithms [3] were applied to explicit atomistic simulations. Potential of mean force profiles were retrieved from equilibrium calculations allowing for discriminating permeable and less-permeable peptides, by employing a relatively affordable computational protocol. Comparing the free-energy differences due to membrane partition and crossing, simulations could be exploited to prioritize peptide modifications. Insights coming from simulations assert some of the properties favoring the membrane permeation.

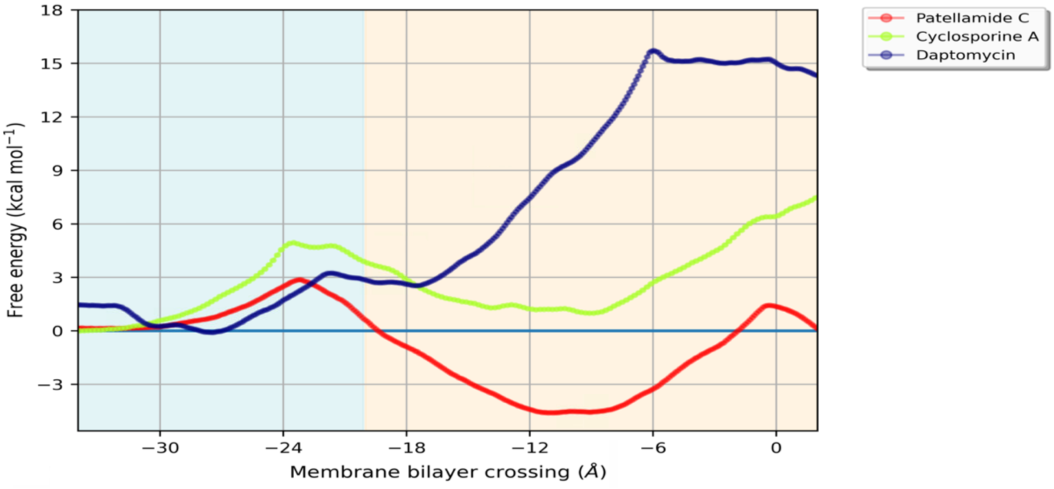

Figure 1: Exemplary potential of mean force profiles representing the process of membrane crossing for cyclic peptides with varying permeability.

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POS42

Gran Sasso National Laboratories as host site of radiobiology experiments: the role of chemistry and mass spectrometry in RENOIR and DISCOVER22 experiments

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In addition to particle and sub-particle physics experiments, the Gran Sasso National Laboratories (LNGS) in Italy have hosted many radiobiology experiments over the years. A recent radiobiology experiment, RENOIR, used the fruit fly *Drosophila melanogaster* as a model organism with the aim of understanding the effects of reduced environmental background radiation on the metabolism of living organisms. RENOIR aims at studying the biophysical mechanisms that trigger the different biological response(s) observed in *Drosophila* reared in the above ground environment (reference radiation environment, RRE) compared to the underground environment (low radiation environment, LRE), where the cosmic ray flux is significantly reduced [1]. Currently another radiobiology experiments started at LNGS, DISCOVER22. The main goal of DISCOVER22 is to understand how the LRE modulates the immune system response in *in vitro* (human cells) and *in vivo (Drosophila)* models.

For these radiobiology studies is mandatory to perform a detailed characterization of the radiation field to which the biological systems are exposed in both LRE and RRE through spectrometric and dosimetric characterization of the environments and the contribution derived from intrinsic radiation of the experimental set-up (i.e., culture medium, plastics and reagents)

The evaluation of the intrinsic ionizing radiation contribution from experimental set-up was carried out by Inductively Coupled Plasma Mass Spectrometry (ICP-MS). To determine total amount of impurities regards to natural radioactive elements (Th, U, K), so intrinsic contribution of radioactivity, High Resolution Inductively Coupled Plasma Mass Spectrometry was used to quantitative analysis of interested elements [2]. Obtained results and relative considerations will be discussed to describe radioactivity of our experimental environments.

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POS43

Multi-elemental analysis of niche celery varieties: exploring the mineral composition of Torricella Peligna black and Trevi black cultivated in an experimental field

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This study aimed to assess the multi-elemental composition of four different celery varieties, with particular emphasis on the characteristic elemental profile of two traditional cultivars [1]. Specifically, the niche celery varieties, Torricella Peligna Black and Trevi Black, are unique black cultivars grown in specific regions of central Italy (Abruzzo and Umbria) and are subject to conservation efforts by the Slow Food Presidia and regional biodiversity registries. All four celery cultivars were grown in an experimental field in Torricella Peligna (Abruzzo) under the same pedoclimatic conditions, with planting in May 2021 and harvesting in December 2021. After appropriate sampling, the celery leaves were harvested, frozen at -18°C, dried at 85°C for 24 hours, and ground. Acid mineralization assisted by microwaves was applied to 20 mg of dried samples, which were analyzed using Inductively Coupled Plasma-Mass Spectrometry (ICP-MS). The accuracy and precision of the analytical method were evaluated through spiking recovery analysis (Figure 1). Various chemometric approaches were employed on a matrix of 70 samples and 14 variables. Principal Component Analysis was used to identify sample trends and assess preferentially bioaccumulated elements, while Covariance Selection-Linear Discriminant Analysis, Partial Least Squares-Linear Discriminant Analysis, and Soft Independent Modelling of Class Analogies, validated through double cross-validation, were utilized to identify the most discriminating elements, evaluating the potential of the multi-elemental profile to differentiate and authenticate the high-value niche varieties from the common ones. This research provides valuable insights into the rediscovered and protected celery cultivars, emphasizing the importance of better understanding the variability and potential value of these niche varieties for promoting biodiversity conservation.

	Na	***Mg***	***P***	***K***	***Ca***	***Sr***	***Al***
Recovery (%)	104	125	99	108	101	101	95
RSD (%)	**2**	**1.4**	**1**	**1**	**3**	**5**	**8**
	B	***Mn***	***Ni***	***Zn***	***Mo***	***Ba***	***Fe***
Recovery (%)	104	101	100	94	102	101	102
RSD (%)	**5**	**3**	**10**	**7**	**5**	**4**	**4**

Figure 1: Relative Standard Deviation of 10 replicates (RSD %) and Recovery (R%).

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POS44

Vapochromic properties of a Zinc(II) salen-type Schiff-base complex for detection of volatile organic compounds

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Volatile Organic Compounds (VOCs) are organic compounds, in liquid or solid form, which, owing to their high vapor pressure, can easily evaporate at room temperature. Some VOCs, used and produced from many manufacturing industries can be hazardous to human-health, and are becoming a major cause of air and ground-water pollution [1]. In this context, the development of simple, low-cost and fast chemosensors, is needed for the direct monitoring of VOCs in specific environments.

Among them, vapochromic molecular materials based on Zn(II) salen-type Schiff-base complexes can represent promising and straightforward chemosensors. In fact, their Lewis acidic character allows to form stable penta-coordinated adducts with VOCs having Lewis basicity. This phenomenon leads to significant color changes with respect to pristine zinc complexes, allowing in-situ detection of volatile organic compounds [2].

In this contribution, we explored the stimuli-responsive chromic properties of a substituted Zn(salen)-type complex derivative from the 2,3-diaminomaleonitrile, Zn(salmal), with 5,5´-tert-butyl-bulky substituents on the salicylidene rings [3]. This complex exhibits distinct thermo- and vapochromic properties (Figure 1). In particular, the anhydrous complex, and related cast films on glass or paper substrates, achieved by solvent evaporation under anhydrous conditions from its tetrahydrofuran solutions, shows a marked vapochromism if exposed to vapors of various VOCs. Interestingly, such vapochromic behavior involves well-defined optical absorptions and distinct naked-eye color changes, also allowing to discriminate primary aliphatic amines.

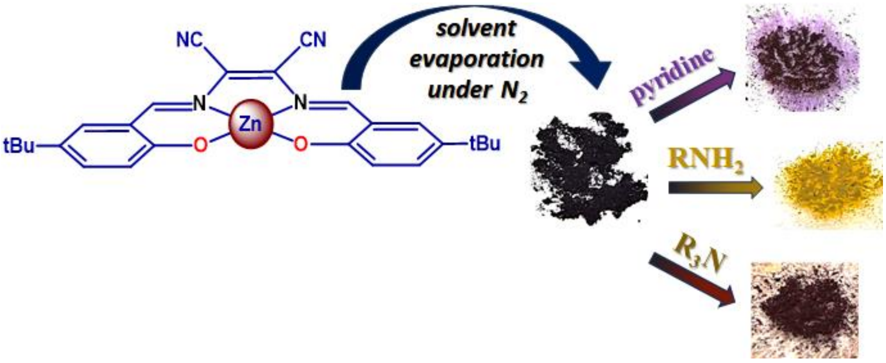

Figure 1: Scheme reporting the vapochromic behavior of our Zn(salen)-type complex.

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

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POS45

Gold-based cytotoxic complexes for targeted anticancer treatments

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In recent decades, the attempts to repurpose auranofin as a possible anticancer agent have triggered growing interest in Au-based complexes as promising candidates in the search for new anticancer therapeutic strategies.[1] Although the mechanism of action for which gold-based compounds cause cellular apoptosis in cancer cells has not been completely clarified yet, it is commonly accepted that the inhibition of thioredoxin reductase (TrxR) plays a pivotal role.[2] At the physiological level, this mitochondrial enzyme maintains the redox homeostasis of the cell, and interestingly it is often overexpressed in tumour cells. Targeting involves the identification of specific molecular biomarkers that are particularly present in cancer cells and the designing of drugs that can interact specifically with them, to obtain a preferential drug's accumulation and selective activity on cancer cells. During the development of this research project, new Au(I)-based complexes were synthesized, characterized, and then conjugated to different molecules able to target cancerous cells, according to different targeting strategies. In particular, three targeting molecules have been implemented in the conjugates. Two gold(I) complexes were firstly conjugated with 2,3,4,6-tetra-O-acetyl-1-thio-β-D-glucopyranose, a biomimetic glucose substrate, potentially able to increase the metal uptake in tumour cells by exploiting the overexpressed GLUT-mediated transport (Warburg effect). Fluorescence and ESI-MS experiments showed the interaction of the new gold(I) conjugates with human serum albumin (HSA), suggesting also the possibility of an HSA-mediated transport in the bloodstream to reach the tumour site. Biological tests on A2780 ovarian cancer cell lines showed a significant enhancement in the cytotoxicity of the complexes when conjugation with 1-thio-β-D-glucose tetraacetate is present. Another approach that has been employed is the conjugation of the same gold(I) complexes with two targeting peptides: C-βAla-RGD, which targets the overexpressed integrin receptors on the A2780 cell line (ovarian cancer), and CrFrFrF, a mitochondria-targeting peptide which allows the drug to accumulate in this organelle, where TrxR is mainly present. During the contribution, the cytotoxicity tests and confocal microscopy experiments will also be discussed.

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POS46

Acyl-CoA dehydrogenase 9 (ACAD9) is a new mitochondrial Complex I (CI) interactor: structural characterization of the CI-ACAD9 assembly and targeted-NMR metabolomics on the ACAD9 substrate palmitoyl-CoA

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NADH-quinone oxidoreductase (Complex I, CI) is the largest and most complicated enzyme complex of the mitochondrial respiratory chain. It is the entry site into the respiratory chain for most of the reducing equivalents generated during metabolism, coupling electron transfer from NADH to quinone to proton translocation, which in turn drives ATP synthesis. The proper assembly of mature CI involves the coordinated assembly of 45 structural subunits. Furthermore, a group of proteins termed assembly factors are required to form the final, mature *holo* complex. Among these factors, the membrane-bound acyl-CoA dehydrogenase 9 (ACAD9) protein has been identified as enzyme in the fatty acid β-oxidation (FAO) metabolic pathway, where it mediates palmitoyl-CoA dehydrogenation, and as a *bona fide* CI assembly factor [1]. While previous studies have shown the association of ACAD9 with CI in mitochondria [2], the molecular mechanisms underlying this interaction remain largely unknown. Given the large range of metabolic diseases caused by CI and ACAD9 deficiencies, a detailed understanding of the macromolecular interactions between both proteins is crucial for our comprehension of the pathogenesis involved and for the development of new therapies for the treatment of such mitochondrial diseases. Here, we present our recent results on the first structural characterization of the CI-ACAD9 assembly. Extensive multidisciplinary approaches (including Small Angle X-ray Scattering, cryo-Electron Microscopy, Electro Paramagnetic Resonance, and targeted-NMR on palmitoyl-CoA) allowed us to provide the first structural and functional analysis of this unique macromolecular complex.

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POS47

Identification of blood transport proteins to carry temoporfin: from virtual screening to PDT testing

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Temoporfin (mTHPC) is one of the most promising photosensitizers used in photodynamic therapy (PDT) for the treatment of the squamous carciroma of head and neck [1]. Despite its clinical use, the lipophilic character of mTHPC still hampers the full exploitation of its potential. The hydrophobicity of mTHPC leads to aggregation, decreasing the long-lived triplet excited state lifetime and consequently reducing ROS production efficiency [2].

This work aims to identify potential dispersing agents among the blood transport proteins through a reverse docking protocol [3]. The computational approach identified apohemoglobin, apomyoglobin, hemopexin, and afamin as the most interacting proteins able to disperse monomolecularly the mTHPC. The computational results were validated through the synthesis of the mTHPC-apomyoglobin complex (mTHPC@apoMb) [3]. The complex preserves the imaging properties of the molecule and improves its ability to produce ROS via both type I and type II mechanisms. mTHPC@apoMb was tested on the CAL27 cell line: upon irradiation, the phototoxicity of mTHPC@apoMyo significantly increases in a concentration-dependent manner [3]. Blood transport proteins can be used as molecular “Trojan horses” in cancer cells by conferring to mTHPC (i) water solubility, (ii) monodispersity, and (iii) biocompatibility, ultimately bypassing the current limitations of mTHPC in clinical use.

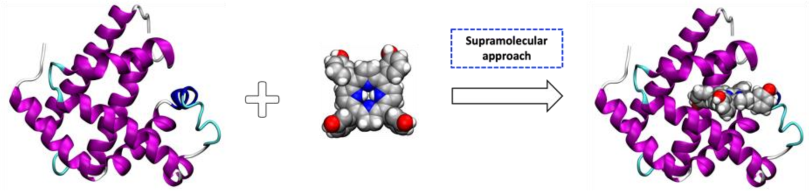

Figure 1: mTHPC@apoMb complex formation.

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POS48

New bimetallic aluminum complexes supported by thioether-amide ligands for ring-opening polymerization of cyclic esters

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The ring-opening polymerization (ROP) of cyclic esters promoted by metal complexes is a synthetic way to prepare aliphatic polyesters. Aluminum complexes are among the most efficient metal initiators for ROP as they exhibit high activity and good control over the polymerization process [1]. More recently, the interest of the research has been direct toward bimetallic aluminum complexes because it was observed that the presence of two close metal atoms within the same complexes can lead to an increase of catalytic activities [2]. The synthesis, characterization and catalytic performances of new bimetallic aluminum complexes are reported in this work where the two metal centers are supported by thioether-amide ligands with thioether-bridge of different lengths. The catalytic performances of each complexes in the ROP of several cyclic esters (L-Lactide, ε-caprolactone and β-butyrolactone) were investigated [3].

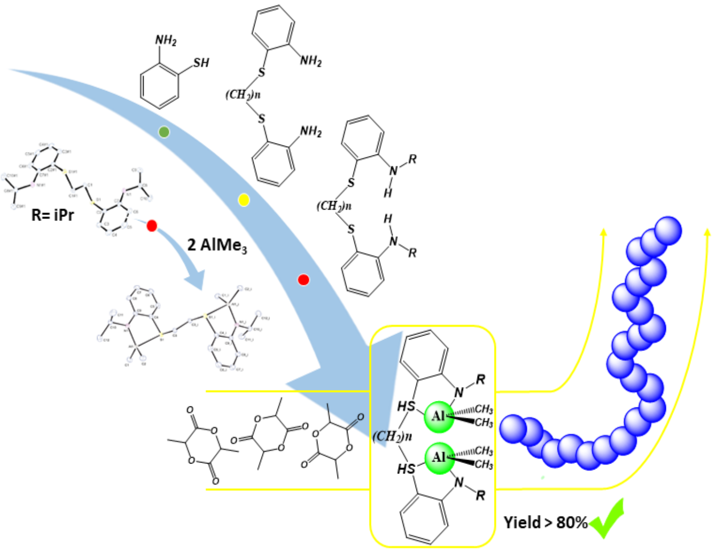

Figure 1: Synthesis of new bimetallic Al complexes and test in ROP

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POS49

Amorphous organic cage forming resistant self-standing membranes with gas permeation properties

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Organic cages are molecules with an internal cavity that can *e.g.* selectively recognize, trap and extract target guests, such as ionic species in aqueous solution and competing media [1]. In the solid state, the packing of these molecules can generate extrinsic and interconnected pores, useful for adsorption or separation applications. Recently, some papers reported the possibility to fabricate membranes of neat organic cages, without the need to add matrix-forming polymers. However, only rare examples of self-standing membranes of neat organic cages are known so far [2].

In this work, the preparation and physico-chemical characterization of a novel organic cage are presented. Thanks to its remarkable film-forming properties, this cage could be solution-processed into transparent thin-layer films and mechanically stable dense self-standing membranes of defined thickness. These peculiar features permitted to determine the mechanical properties and to test these membranes for gas permeation, reporting a behaviour similar to that of polymers of intrinsic microporosity. Moreover, the self-standing membranes showed a good chemical stability (if properly stored in a desiccator, away from moisture) over a period of two months. Considering the growing interest in the development of film-forming molecular systems suitable for separation technologies and functional coatings, the properties of this organic cage were investigated by thorough analysis of their structural, thermal, mechanical and gas transport properties, and by detailed atomistic simulations [3].

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POS50

Sustainable exploitation of dried fruit hard shells for the development of novel anti-diabetic ingredients

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Type 2 diabetes mellitus (T2DM) is a chronic metabolic disorder characterized by high blood glucose levels. Its pathogenesis is strongly correlated with oxidative stress induced by the increase of radical oxygen species (ROS) [1]. One of the therapeutic approaches to control postprandial hyperglycemia in T2DM is inhibiting the digestion of dietary carbohydrates, delaying the glucose uptake and, consequently, reducing the blood sugar levels. Although some drugs inhibit α-glucosidase and α-amylase, they produce many side effects, leading to the research of new inhibitors [2].

Pistacia vera, *Prunus dulcis* and *Corylus avellana* hard shells are underexploited agri-food waste that have the potential to be further processed into new value-added nutraceutical ingredients, constituting a valid alternative to synthetic drugs [3]. In the present study, valuable bioactive compounds were recovered from *P. vera*, *P. dulcis* and *C. avellana* dried fruit hard shells by using an optimized microwave-assisted extraction (MAE) protocol. The inhibitory activity against α-glucosidase and α-amylase, as well as the antiradical activity against ROS were *in vitro* evaluated. Mass spectrometric analysis was conducted to elucidate the phytochemical composition of the extracts. Furthermore, cell viability assays were performed to assess the safety of the optimized extracts on two human intestinal cell lines (HT29-MTX and Caco-2).

This work demonstrates the potential of dried fruit hard shells for the development of new potential dual-action anti-diabetic ingredients, able to reduce postprandial hyperglycemia and prevent cellular damage induced by ROS.

Figure 1. Valorization of dried fruit hard shells.

[1] G. Davì, F. Santilli, C.Patrono. *Cardiovascular Therapeutics*. 28 (2010) 216-226
[2] N. Cardullo, G. Floresta, et al. *Bioorganic Chemistry*. 117 (2021) 105458
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POS51

Ultrasound-assisted extraction of tomato waste using extra virgin olive oil as solvent

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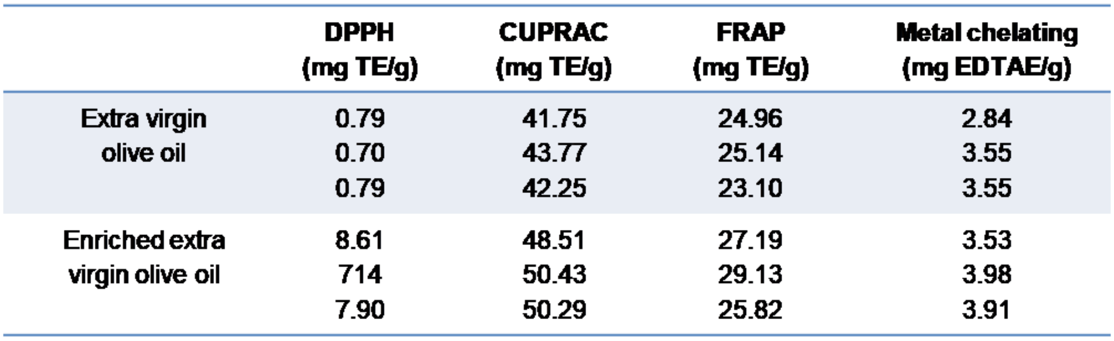
Tomatoes are known as a rich source of lycopene (especially tomato peels). Lycopene is a carotenoid that shows a natural antioxidant effect. With the aim to revaluate tomato wastes, like peels, stems and seeds, we tried to enrich extra virgin olive oil with lycopene using a completely green approach.

Considering the hydrophobic nature of carotenoids, an ultrasound-assisted extraction has been performed using extra virgin olive oil directly as solvent due to its high lipophilic nature. Lycopene was then quantified by HPLC-DAD using the method proposed by Olives Barba *et al.* [1], with slight modifications. Then the results were compared with the lycopene yield obtained extracting with conventional organic solvent.

The antioxidant activity was determined before and after the process of extraction. As we can see in Figure 1, DPPH assay shows a substantial increase of the antioxidant activity after the enrichment process. CUPRAC and FRAP assays displays a slight improvement of antioxidant activity. On the contrary, metal chelating activity is pretty the same.

This preliminary work can be the starting point for the production of new kind of enriched food using food wastes leading to the consequent reduction of the food industrial environmental impact.



	DPPH (mg TE/g)	CUPRAC (mg TE/g)	FRAP (mg TE/g)	Metal chelating (mg EDTAE/g)
Extra virgin olive oil	0.79	41.75	24.96	2.84
	0.70	43.77	25.14	3.55
	0.79	42.25	23.10	3.55
Enriched extra virgin olive oil	8.61	48.51	27.19	3.53
	714	50.43	29.13	3.98
	7.90	50.29	25.82	3.91

Figure 1: Comparison between the antioxidant activity of the extra virgin olive oil before and after the extraction procedure.

[1] A.I. Olives Barba, M. Cámara Hurtado, M.C. Sánchez Mata, V. Fernández Ruiz, M. López Sáenz de Tejada, *Food Chemistry* 95 (2006) 328–336

POS52

Turning the light on with pyrazolo[1,5-A]pyridine: exploring it's fluorescent properties for the design of new fluorosteric compounds

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Receptor target fluorescent probe is an imaging technique used to studying and understanding biological processes in live organisms [1]. However, the alteration of the pharmacological and physiochemical characteristics of the biological ligand is a significant drawback of this method. To avoid these issues, one potential strategy involves merging the concepts of biological target and fluorescent probe, resulting in the design of a biologically active fluorescent ligand [2].

Pyrazolo[1,5-a]pyridin-2-ol is a small molecule characterized by a strong emission in the blue field. Its physicochemical features as carboxylic acid isostere have been highlighted in MEDS433, a potent *h*DHODH inhibitor. [3]. With the purpose of moving the emission profile from blue to red while keeping the scaffold's modest size, two series of compounds were design. In the first series, a yellow-red bathochromic shift was achieved by increasing the π-conjugated network of the scaffold, that was, however, accompanied by a low quantum yield. In the second series, a scaffold rigidification was used to achieve a yellow-red bathochromic shift and an adequate quantum yield.

Here, the comprehensive analysis of the fluorescence properties of this probe, as well as the first biological application achieved by design a new *h*DHODH inhibitor, will be discussed.

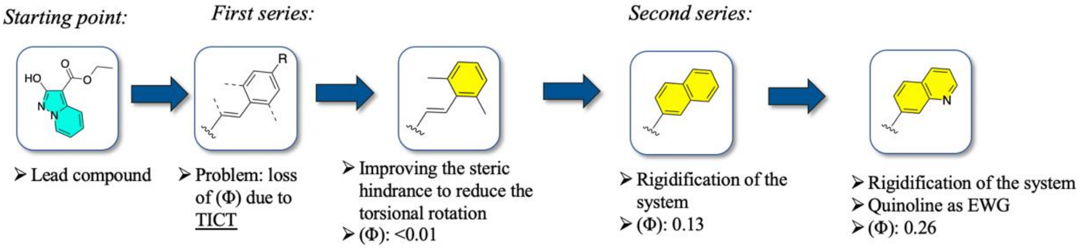

Figure 1: The image above provides a summary of the fluorescence probe's design.

[1] Xia, T., Li, N., & Fang, X. Annual Review of Physical Chemistry, (2013), 64(1), 459–480.
[2] Joomyung V. Jun, David M. Chenoweth and E. James Petersson, Org. Biomol. Chem., (2020), 18, 5747
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POS53

Effect of Sn (or Sb) precursor in Fe-N_x site formation and activity in Fe-N-C catalyst for ORR

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The expansion of the market for fuel cells that rely on platinum-based catalysts is constrained by the high cost and limited availability. Nitrogen and iron-doped carbon material (Fe-N-C), has been extensively researched as an alternative, focusing on understanding the nature, formation, stability, and reaction mechanism of the active sites. Being Fe-N-C materials complex, bimetallic systems have received less attention. Recent examples use Fe coupled with Ni, Mn, or Cu. In certain cases, the bimetallic system shows better performance and stability but there are examples of worst activity due to Fe site formation inhibition. So far, only a few papers report on the use of *p*-block metals, such as Sn [1]. Motivated by these findings and based on our prior research [2], we have chosen to study bimetallic systems containing Fe and Sn (or Sb). Here we will present the latest results by using different Sn (or Sb) precursors to see the impact on SnN_x formations and ORR activity and selectivity. The catalysts were synthesized by a typical thermal synthesis starting from carbon black and metal-nitrogen complexes. RRDE and GDE techniques in acidic and alkaline electrolytes were used to evaluate the selectivity, activity, and stability towards the 4e-ORR. XAS (Figure 1), TEM, SEM, and XRD were used to evaluate the effect of different Sn (or Sb) precursors on fixed phases. The bimetallic catalysts exhibited an improvement compared to the monometallic Fe, which can be attributed to the presence of Sn-N_x. NO_2 stripping shows that the SD grows linearly with the bulk content of nitrogen, suggesting a predominance of Fe-N_x sites over Sn-N_x. *In-situ* measurements were done on Sn/Fe-N-C at both Fe and Sn K-edge (Figure 1b-d). For iron, there is an oxidation state variation during potential cycling, but not for Sn.

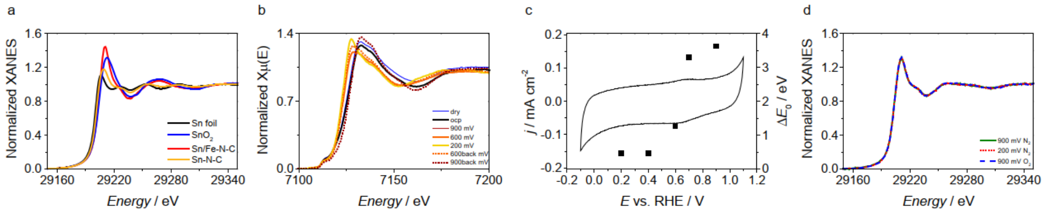

Figure 1: a) Ex-situ measurement for Sn and Fe/Sn-N-C on Sn K-edge, b) variation of Fe K-edge response under applied potential, c) variation of edge as a function of potential, overlapped with CV, and d) response under potential variation for Sn K-edge.

[1] F. Luo, A. Roy, L. Silvioli, D.A. Cullen, A. Zitolo, M.T. Sougrati, I.C. Oguz, T. Mineva, D. Teschner, S. Wagner, J. Wen, F. Dionigi, U.I. Kramm, J. Rossmeisl, F. Jaouen, P. Strasser, Nat. Mater. 19 (2020) 1215–1223.
[2] M. Mazzucato, L. Gavioli, V. Balzano, E. Berretti, G.A. Rizzi, D. Badocco, P. Pastore, A. Zitolo, C. Durante, *ACS App. Mater. Interfaces.* 14 (2022) 54635–54648.

POS54

A new way to surface functionalize nanostructured *magnetorheological electrolytes* with the use of click-chemistry

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Today, more than ever, the interest in the reduction of pollution and waste, and in the displacement of fossil fuels is high. REMAP (Reusable Mask Patterning) [1] is a project funded by the European Union that wants to revolutionize the microfabrication sector (e.g. for advanced photovoltaic applications) by developing a greener surface patterning technique. REMAP's basic idea is to design so-called *magnetorheological electrolytes* (MREs) [2], fluids based on magnetic nanoparticles (NPs) and electrolytes that modify their apparent viscosity upon modulation of microstructured magnetic field gradients onto a substrate. Specifically, we are crafting the MRE properties to form infinitely reusable masks that would represent a huge step forward in the field of microfabrication with respect to standard lithography.The following key factors must be fulfilled for the intended application: i) high masking efficiency, ii) colloidal stability in aqueous media, and iii) fast redispersion of NPs in the absence of a magnetic field gradients. To obtain this, we decided to create organic custom-made ligands that can be covalently bound to the surface of NPs using click-chemistry to drastically change the surface properties of NPs (*figure 1*).

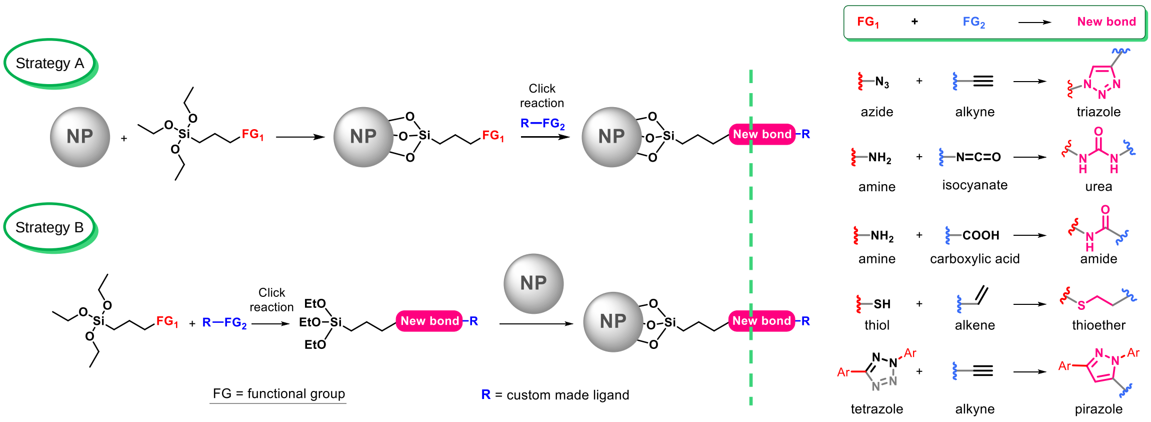

Figure 1. Possible strategies and click reactions that can be used for the surface functionalization

Herein, we present the design and the synthesis of the organic ligands, and their application in the surface functionalization of NPs.

1. https://re-map.eu/.
2. K. Shu., C. Wang, W. Li, T. Bussell, J. Ding, *Current Opinion in Electrochemistry,* 2020**,** *21*, 297-302

POS55

Elsevier’s chemistry ecosystem

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The chemistry ecosystem at Elsevier consists of an extensive network of resources: scientific journals, books, and digital tools that serve researchers, academics, experts and professionals in the field of chemistry. Among these resources we can highlight:

- SciVal, a research performance analysis tool useful to understand the research landscape, provide insights into area trends, identify top-performing researchers and institutions, and understand funding sources that support research in the field.
- Scopus, a comprehensive abstracting and indexing database where researchers can explore and discover scientific literature, track citations, and identify key authors and institutions contributing to specific topics.
- Elsevier's eBooks collection, including a vast array of chemistry-related books and reference material.
- Reaxys [1], the premier chemistry database providing access to a wealth of chemical information, including compounds, reactions, and properties, essential to explore the chemical space, plan synthetic routes, and access curated experimental data.
- PharmaPendium [2], a pharmacology database containing regulatory information, drug safety data, and clinical outcomes, that help researchers understanding potential bioactivity and the effects of drugs or compounds on biological pathways.
- Embiology and Embase [3], two biomedical databases that can be used to monitor adverse reactions to specific compounds and/or to gain insights into potential implications on biological pathways and protein regulation.

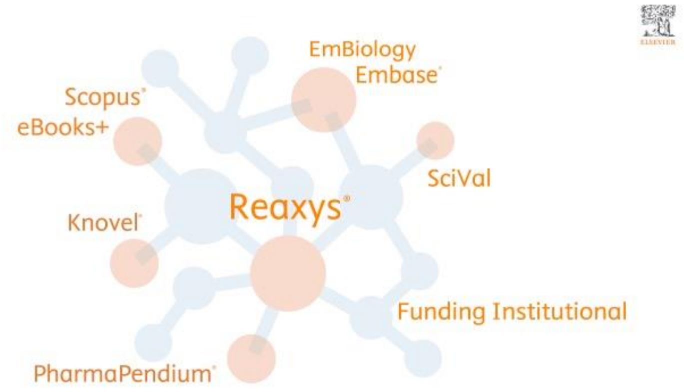

Figure 1: The Elsevier’s Chemistry Ecosystem tree.

[1] https://www.elsevier.com/solutions/reaxys
[2] https://www.elsevier.com/solutions/pharmapendium-clinical-data
[3] https://www.elsevier.com/solutions/embase-biomedical-research

POS56

Ironing out Fe^{3+} acquisition in *M. abscessus*: a new strategy to target virulence factors in non-tuberculous mycobacteria

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M. abscessus (*Mab*), which belongs to the class of non-tuberculous mycobacteria (NTM), is an opportunistic pathogen that causes chronic pulmonary infections in sensitive individuals, especially cystic fibrosis (CF) patients. Due to the intrinsic resilience of NTM to the available treatments, which is worsened by the dramatic spread of resistant strains, new therapeutic strategies are urgently needed [1].

In this context, iron acquisition has recently emerged as an interesting target in the phylogenetically close *M. tuberculosis* (*Mtb*), due to the involvement of this metal in the pathogenesis and survival of the microorganism in the host [2]. Hence, we investigated the targeting of mycobacterium-specific iron chelators as a possible anti-virulence approach against *Mab*. In detail, we focused on the first enzyme involved in the siderophore biosynthetic pathway, a salicylate synthase (SaS) that has been successfully studied to identify antitubercular agents against *Mtb*. Due to the structural conservation of the active site in the two congeners, we approached this study by screening an in-house library of *Mtb*-SaS inhibitors. This initial investigation led to the identification of the first hit compounds against *Mab*-SaS. Their activity was rationalized using a homology model, based on the PDB coordinates of the *Mtb* protein [3]. However, considering the high plasticity of the active site and the flexibility of two loops adjacent to the binding cavity, we decided to perform crystallization studies to solve the structure of *Mab*-SaS, thus providing a solid base to structure-based drug design efforts. The obtaining of the first 3D-model of this enzyme allowed us to characterize its orthosteric site and study the peculiar area around it. Our preliminary but promising results will be presented, along with perspectives on the use of the new structure for the development of optimized inhibitors.

[1] A. van Dorn, *Lancet Respir. Med.* 5 (2016) 1-15.
[2] G. Stelitano, M. Cocorullo, M. Mori, S. Villa, Fiorella Meneghetti, and L. R. Chiarelli, *Int. J. Mol. Sci.* 24 (2023) 6181.
[3] M. Mori, G. Stelitano, G. Cazzaniga, A. Gelain, A. Tresoldi, M. Cocorullo, M. Roversi, L. R. Chiarelli, M. Tomaiuolo, P. Delre, G. F. Mangiatordi, A. Griego, L. Rizzello, A. Cassetta, S. Covaceuszach, S. Villa, and F. Meneghetti, *Pharmaceutics* 15 (2023), 502.

POS57

Quantification of fatty acids in biological samples using vacuum-assisted headspace-solid phase microextraction

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There are variety of studies about dietary fatty acids and trans fatty acids in food source, food intakes and various biological samples such as blood and faces. It appears that high levels of some fatty acids or significant differences in their ratio indicate a variety of diseases (i.e., cancer, diabetes etc.)[1]. Regarding the analysis of fatty acid, attention is required to accurately measure the amount of trans and cis isomers. Even though LC-MS seems to be suitable for separation of long chain fatty acids, the usage of GS-MS is more common due to better sensitivity. Whereas short chain fatty acids and some medium chain fatty acids (up to C10) can be analysed directly, long chain fatty acids (LCFAs) require derivatization. The most common way is esterification to form fatty acid methyl esters (FAMEs). However, analysis of trans fatty acid might be challenging for the incomplete separation of cis and trans FAMEs, poor sensitivity, and double bond isomerization. Head space solid phase microextraction (HS-SPME) is known as a fast and effective method for sample preparation. Some research shows that using vacuum may lead to improve transfer of the analytes from sample to gaseous phase and reach equilibrium or at least increase the signal faster and at lower sorption temperature [2].

In this research, for the first time, a vacuum-assisted HS-SPME (Vac-HS-SPME) GC-MS method was developed for determination of more than 25 fatty acids in faecal and serum samples. Derivatization to FAMEs was applied for LCFA analysis. All the steps of the analysis as extraction, derivatization, Vac-HS-SPME were investigated to increase the signal and preserve the original concentration and ratio of fatty acid. Design of Experiments (DoE) concept was applied to optimize the analytical method. As an advantage, our vacuum system was not tailored design [3], but we used commercially available tools. By comparing the optimized Vac-HS-SPME and regular HS-SPME procedures we proved that Vac-SPME method was more sensitive, with lower limits of detection (from 0.05 to 10 µg L-1) than regular HS-SPME for almost all target analytes. Intra- and inter-assay precision CVs were ⩽9.0% and ⩽12.5%, respectively. The Vac-HS-SPME method was successfully applied to quantify FAs in samples of 10 healthy subjects.

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[3] M.J. Trujillo-Rodriguez, V. Pino, E. Psillakis, J.L. Anderson, J.H. Ayala, E. Yiantzi,and A.M. Afonso, *Analytica Chimica Acta,* 962 (2017), 41-51.

POS58

Multivalent iminosugars targeting the levansucrase enzyme as a new plant protection strategy against kiwifruit canker

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[b] *Dipartimento di Scienze Biomediche Sperimentali e Cliniche “Mario Serio” (SBSC), Università degli Studi di Firenze, Viale Morgagni 50, 50134-Firenze, Italy*
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Since few years the Italian crops of kiwifruit are devasted by a bacterial canker disease caused by *Pseudomonas syringae pv. actinidiae* (Psa) biovar 3. In this bacterium, the enzyme levansucrase is deputed to the synthesis of levan, a hexopolysaccharide involved in the survival strategies of many different bacteria [1]. For these reasons, the identification of new compounds able to inhibit the levansucrase enzyme is an important target. Two putatively functional levansucrases were cloned and expressed in *E. coli* by some of us and their biochemical properties characterized [2]. The enzyme catalyses both the hydrolysis of sucrose and the levan polymerization. We selected a non-toxic pyrrolidine iminosugar ring (1,4-deoxy-1,4-imine-D-arabinitol (DAB-1)), derived from an inexpensive sugar (D-arabinose), whose multimerization on a di-, tri- or a tetravalent scaffold (e.g. compound **1**, Figure 1), resulted in the inhibition of both hydrolytic and polymerising enzyme activities [3]. We report our synthetic efforts aimed at the synthesis of the PEG-ylated analogue of **1**, namely compound **2**, which should be more soluble in water thus avoiding bioaccumulation, in view of future potential application as an agrochemical for crop protection.

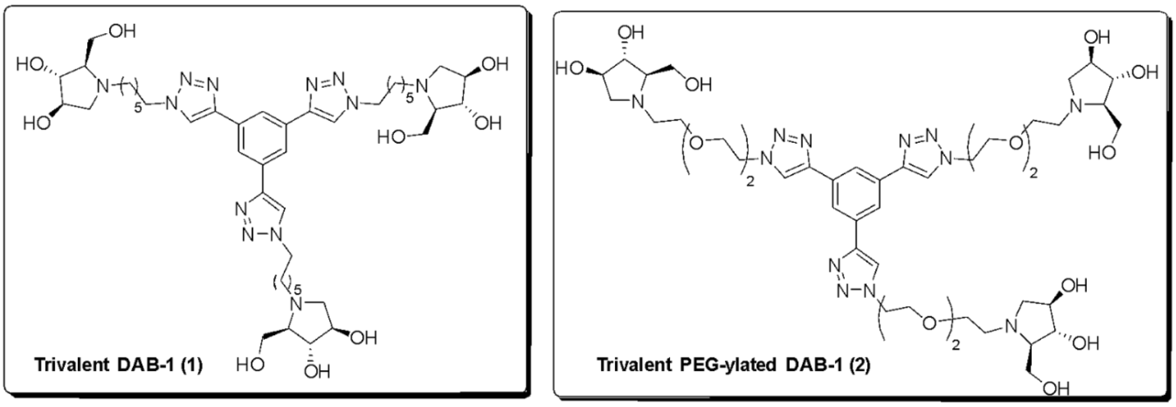

Figure 1: Trivalent DAB-1 (**1**) and its PEG-ylated analogue **2**.

[1] S. Kasapis.*et al. Carbohydr. Polym. 23,* (1994) 55
[2] S. Luti *et al., Int. J. Biol. Macromol. 179*, (2021) 279
[3] A. Berto, Tesi laurea triennale in chimica, Università degli studi di Firenze (2022) Relatore: Prof. Dr. Francesca Cardona, Correlatore: Dr. Francesca Clemente

POS59

Glassy poly-4-chlorostyrene isenthalpic evolution: evidence of secondary mechanism assisting α-relaxation dynamics

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The decrease in free energy of an out-of-equilibrium system is commonly mediated by molecular relaxation processes, which result from spontaneous rearrangements at molecular level [1]. In the context of glassy materials, the gradual evolution of thermodynamic properties in a non-equilibrium glass, known as physical aging, is usually described invoking the exclusive role of the super-Arrhenius α-relaxation [2]. In this study we investigated the enthalpic relaxation kinetics of atactic poly-4-chlorostyrene P4ClS after temperature down-jumps in the glassy state across a broad temperature range. Fast scanning calorimetry (FSC) was employed to measure both physical aging and molecular mobility. Figure 1a and 1b display the c_P curves and the enthalpic recovery during the isothermal aging of P4ClS at two different temperatures, namely 390 K and 406 K. In the experiment conducted at 406 K, the overshoot stabilizes simultaneously with the plateau of the enthalpic recovery at a time scale compatible with the exclusive role of the α-relaxation. In contrast, aging performed at 390 K exhibits approach to a plateau in the enthalpy with time scales vastly deviating from that of the α-relaxation; followed by further isenthalpic evolution of the endothermic overshoot mediated by the α-relaxation. As evidenced on the Arrhenius plot in figure 1c, these findings suggest the existence of an additional molecular mechanism assisting the α-relaxation in the physical aging.

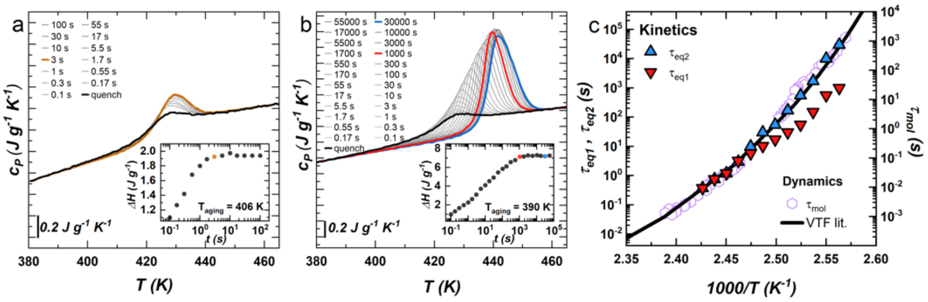

Figure 1: P4ClS c_P curves and enthalpic recovery for isothermal aging at 390 K (a) and 406 K (b). Arrhenius plot (c)

[1] Z. Song, C. Rodrìguez-Tinoco, A. Mathew and S. Napolitano, *Sci. Adv. 8* (2022) eabm7154
[2] P.G. Debenedetti, and F.H. Stillinger, *Nature 410* (2001) 259-267.

POS60

Electronic current densities and origin-independent property densities induced by optical fields

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The interaction of a molecule with optical fields is customarily interpreted by means of induced time-dependent electric polarizabilities, magnetizabilities and mixed electric-magnetic polarizabilities. In general, these properties can be rationalized by integrals of density functions formulated in terms of induced charge and current densities. Here, we focus on what has been done so far at theoretical level, and on what can be expected to be unveiled from the topological study of suitable density functions, endowed with the fundamental requirement of origin invariance. Densities characterized by such a property can be integrated all over the configuration space to obtain electric dipole polarizability and optical rotatory power. Corresponding maps visualize domains mainly involved in the molecular response. The diagonal components of origin-independent density tensor functions have been computed, confirming the ubiquitous presence of counter-polarization regions in the proximity of the atomic nuclei. They are associated with toroidal electron currents, induced by time derivative of the electric field of impinging radiation. Electron (de)localization in these systems is readily observed and estimated. The optical rotation density of the carbonyl chromophore is studied in detail. Its essential feature is the separation in quadrants of alternating sign of the density about the CO bond. The presence of an extrachromophoric perturbation determines asymmetry in the extension of the quadrant distribution, thus causing optical rotation.

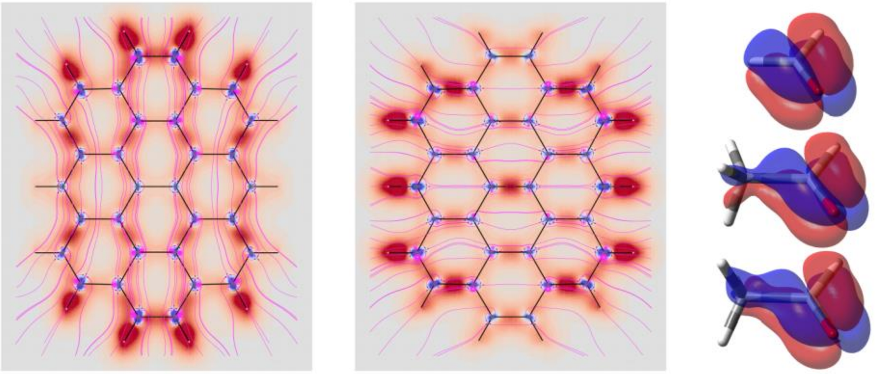

Figure 1: Left and center: in-plane components of electric dipole polarizability density for ovalene over the molecular plane; trajectories of the current density induced by the time derivative of the electric field are superimposed. On the right: specific rotation power density: top formaldehyde; middle acetaldehyde with achiral conformation; bottom acetaldehyde with chiral conformation. Iso-surfaces are $\pm$100 deg[dm g/cm^3]$^{-1}$a$_0^{-3}$ Red/blue positive/negative vales.

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POS61

Metabolomics and NMR for the rapid identification of potential anticancer compounds

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Cancer is a rapidly spreading deadly disease. Despite advances made in the medical and clinical fields, approximately 7 million people die each year. Therefore, the discovery and/or development of novel anticancer drugs is important.

In this field the potential of natural products and their derivatives is considerable because of their significant structural diversity as well as pharmacological and molecular features[1].

So, in this work, twelve Asteraceae plant extracts have been screened in the search for metabolites that can be used in the treatment of colorectal cancer as non-invasive therapy. The metabolomic approach, by means of nuclear magnetic resonance (NMR), and biological activity assays were combined in order to select the most interesting extracts. The application of NMR spectroscopy methodologies as a non-invasive and non-disruptive technique, allowed significant improvements in the identification of natural products, representing a powerful tool that allows a high-resolution description of the structure of each individual component contained within crude extracts[2]. On the other side, biological assays performed on a panel of human colorectal cancer cell lines allowed to screen the biological activity of the extracts enriched in specialized metabolites.

Based on the data analysis of the results, five plant extracts, i.e., *Anthemis maritima*, *Artemisia vulgaris*, *Centaurea deusta*, *Erigeron sumatrensis* and *Xanthium strumarium* were selected for further investigation. Therefore, to identify their potential active components directly in the mixture, advanced NMR experiments (PSYCHE, PS- *ed*HSQC, *sel*-TOCSY, DOSY) were applied limiting both time and, above all, cost of classic bio-guided fractionations [3]. As a result, a γ-pyrone derivative, five sesquiterpene lactones were identified. An *ad hoc* phytochemical strategy allowed to rapidly isolate and characterize through 1D and 2D NMR (COSY, HSQC, H2BC, HSQC-TOCSY, CIGAR-HMBC, TOCSY and NOESY) experiments the potential cytotoxins.

The results of these studies encourage further *in vitro* evaluation and mechanisms of action investigation of isolated compounds.

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POS62

A new generation of AKR1C3 inhibitors on the horizon: the 3-hydroxybenzazole approach to target prostate cancer

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Aldo-Keto Reductase 1C3 (AKR1C3) has a key role in androgen biosynthesis, thus an increasing number of studies have focused on AKR1C3 inhibitors for their potential application in treating *Castration-Resistant Prostate Cancer* and preventing drug resistance [1]. Since *flufenamic acid* (FLU, Figure 1) is known to inhibit AKR1C3 in weak and non-selective mode, we employed in recent years a conformational restriction strategy on FLU anthranilic core to afford a bioisosteric 3-hydroxybenzoisoxazole-scaffold based series of compounds [2].

Thanks to the binding pose of the *lead* compound **1** inside AKR1C3 enzyme, determined through X-ray crystallography [2], we designed the next optimized round of *hydroxybenzazole* derivatives, where the B-ring is modulated by further substituents with the purpose of increasing potency and retaining selectivity through a deeper exploration of AKR1C3 binding pocket (Figure 1). *In silico* design, synthesis, *in vitro* biological evaluation (enzymatic and cellular assays) and X-ray structures of the new AKR1C3 inhibitors are here described and discussed.

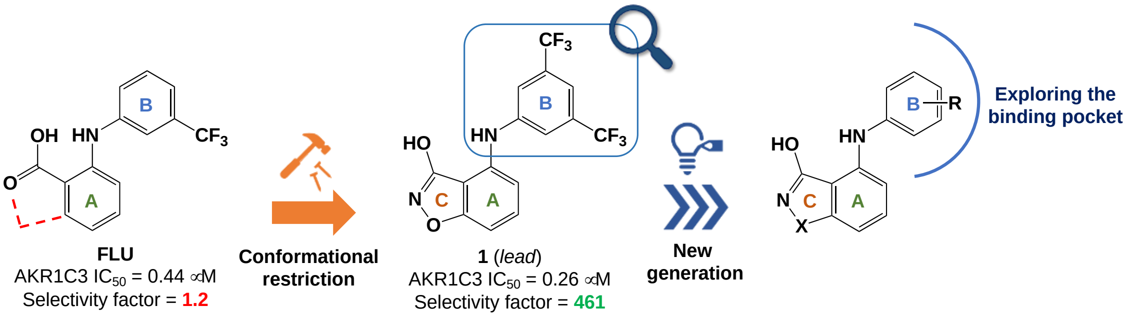

Figure 1: The employed bioisosteric strategy and the suggested modulations of **1**.

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POS63

Modified gold screen-printed electrodes for toxic heavy metals detection

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The health risks associated with toxic metals, even at very low concentrations, underline the need for accurate and efficient sensing technologies.[1] Electrochemical detection based on screen-printed electrodes (SPEs), allows for simple and rapid in-situ monitoring of microvolumes of water-based samples, with high reproducibility, sensitivity and selectivity.[2] The work electrode of these devices can be opportunely functionalized with sensitive elements able to selectively detect contaminants in water.[2] We have synthesized molecules with 1,2,3- triazole structure, containing amino or α-aminophosphonic groups, with high chelating abilities combined with significant selectivity towards highly toxic heavy metal ions, such as Hg^{2+} and Pb^{2+}.[3] The gold surface of gold screen-printed electrodes (SPGEs) was chemically modified using thiol compounds able to form stable gold-sulphur (Au-S) bonds and to covalently bind the synthesized selective ligands. The electrochemical performance of the modified SPGEs was investigated by square wave anodic stripping voltammetry (SWASV) for the detection of Hg^{2+} and Pb^{2+} either alone or in their mixtures.

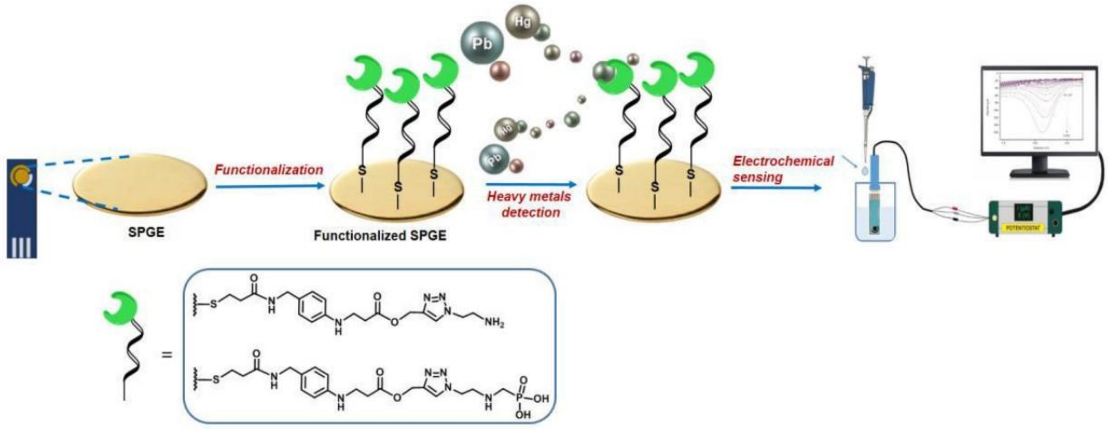

Figure 1: Modified SPGEs for electrochemical monitoring of heavy metals in water.

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POS64

'Flexible dithienyl probes for determining the absolute configuration of chiral molecules'

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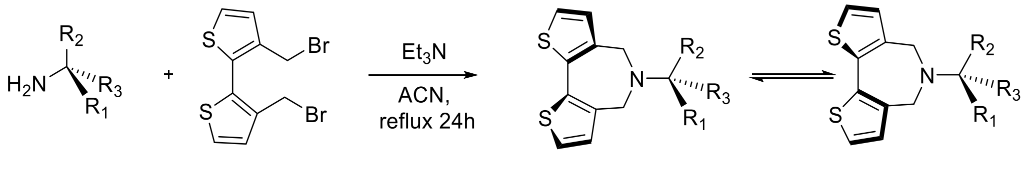
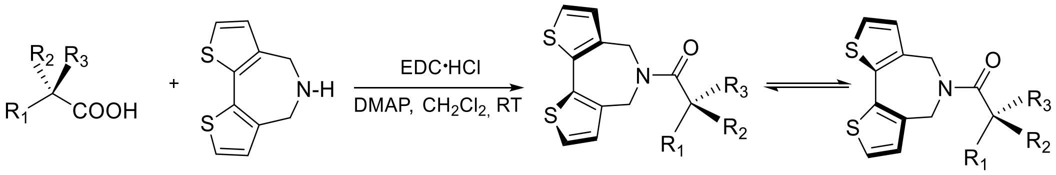
The assignment of absolute configuration is a fundamental task to be addressed when dealing with chiral molecules. To this end, several approaches are now available, like chemical correlation, X-ray analysis, and chiroptical spectroscopy. In particular, the latter approach is particularly appealing, allowing the absolute configuration assignment in short time, in solution, and requiring sub-milligram samples. This allows to treat even compounds not-crystalline and available in very small amounts, like natural products. In recent years, the use of the so-called *chiroptical probes* is emerging as an innovative alternative to the computational methods for chiroptical analysis, particularly in case of conformationally flexible and/or UV-transparent molecules. In this field our group described the application of chiroptical probes based on flexible biphenyls for the assignment of absolute configuration of chiral diols, [1] carboxylic acids, [2] and amines, [3] eventually applying them even to complex natural products. In this communication a novel flexible dithienyl probe is described and applied to determine the absolute configuration of chiral amines, acids and aminoacids. When the amine is transformed in the corresponding dithienyl azepine (Figure 1) a preferred *M* or *P* twist is induced by the chiral substrate depending on its absolute configuration. The preferred twist can be detected by a diagnostic band in the electronic circular dichroism (ECD) spectrum, thus arriving at the absolute configuration of the derivatized amine by the ECD spectrum of the azepine. The same situation occurs when a chiral carboxylic acid is transformed into the corresponding dithienyl amide (Figure 2). The dithienyl probe has the advantage over the biphenyls to provide a more clearly detectable diagnostic ECD signal and to potentially allow absolute configuration assignment even by Optical Rotation measurements.



1 2 ***(M)***-3 ***(P)***-3

Figure 1: Dithienyl probes used for amine absolute configuration determination.



4 5 ***(M)***-6 ***(P)***-6

Figure 2: Dithienyl probes used for carboxylic acids absolute configuration determination.

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POS65

Investigation on the anti-inflammatory properties of hazelnut kernel, skin and leaves through computational techniques

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Hazelnuts and their derivatives have undergone extensive research due to their high content of phenolic compounds, flavonoids, tannins, polysaccharides, and dietary fibers, all of which possess robust antioxidant properties and exhibit various potential health benefits. Numerous studies have highlighted the significant advantages of incorporating hazelnuts into one's diet in terms of managing cardiometabolic risk factors, often exceeding expectations. Furthermore, other research has demonstrated that hazelnut consumption may lower the risk of conditions such as coronary heart disease, atherosclerosis, and specific types of cancers [1].

Our current research focuses on identifying potential targets associated with hazelnut components and their potential roles in these diseases. To achieve this goal, we performed a structure-based virtual screening on a database which collect chemical compounds found in the kernel, skin and leaves of hazelnuts. This approach, involving the assessment of hazelnut constituents on various anti-inflammatory targets, holds great promise as an in silico tool for rational target identification and pharmacological profiling of individual chemical compounds in the realm of natural product research. To verify the predicted theoretical activities, we will carry out in vitro experiments.

Our analysis could provide a valuable strategy for optimizing the utilization of hazelnut by-products in various fields, including nutraceutical and pharmaceutical, ultimately benefiting the scientific community. This work is founded by a CRISEA Research Project [2].

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[2] CUP D13D18000120002 96626238BE.

POS66

Laser-induced graphene electrochemical aptasensor for the detection of *Escherichia coli*

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The detection and identification of pathogenic microorganisms is of crucial importance as they pose a major threat to worldwide health system as well as an economic burden. In the recent years, the advancements in material science have brought to light a novel, interesting material called, Laser-Induced Graphene (LIG), that has attracted interest due to properties that include: its mechanical resistance, its high surface area, and the relative ease in terms of production processes [1]. These characteristics have opened possibilities to develop low-cost and portable electrochemical devices that can respond to point-of-care applications. In this work, a LIG electrode (Fig. 1A) covalently functionalized with two different aptamers (P12-55 and P12-31 [2]) was used for the development of an aptasensor for the detection of E. coli. Electrochemical impedance spectroscopy was used to evaluate the change in the charge transfer resistance of the aptasensor upon interaction with the bacterial cells. The aptasensor showed a linear response in the presence of E. coli within $10^0 - 10^2$ CFU/mL when tested in phosphate buffer saline solution. Importantly, the biosensor proved to be selective for E. coli and negligible response was observed in presence of Staphylococcus aureus and Pseudomonas aeruginosa. Finally, the sensor was calibrated in urine samples spiked with a known concentration of E. coli cells (Fig 1B).

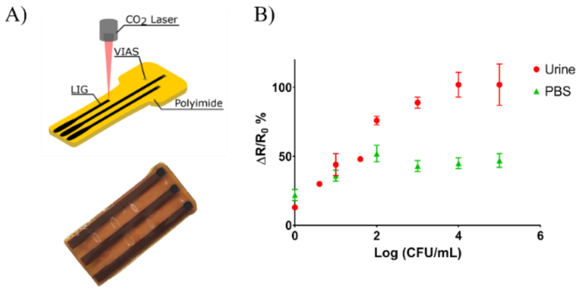

Figure 1: A) LIG electrodes scribed on polyimide. B) Calibration curves at increasing concentration of E. coli in phosphate buffer saline and in urine.

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[2] Marton S., Cleto F., Krieger M.A., Cardoso J., PLoS ONE. 11 (2016) e0153637.

POS67

Unusual antioxidant effect of natural proaromatic terpenes in liposomes

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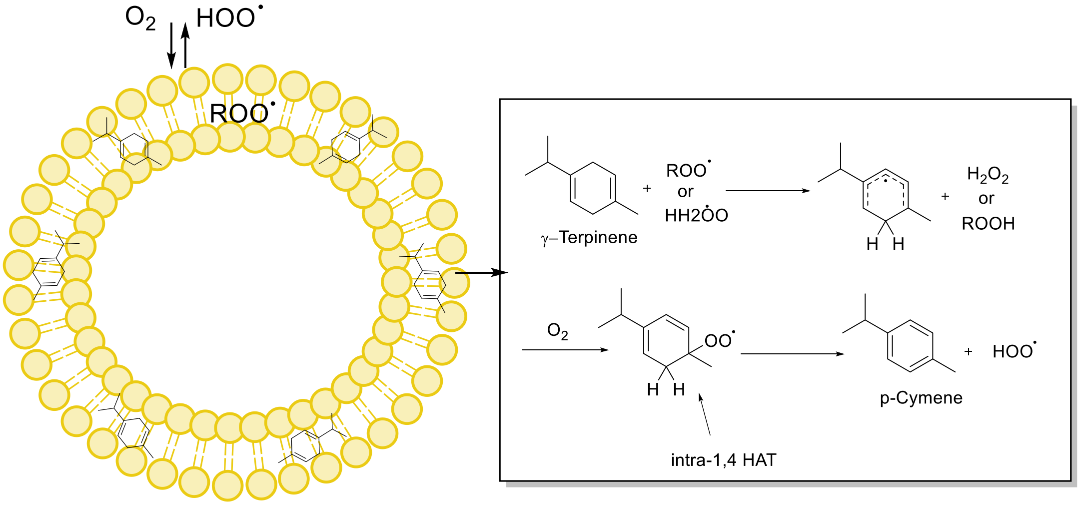
The process of organic compounds reacting with oxygen under mild conditions to form hydroperoxides and other oxygenated compounds is known as autoxidation. Autoxidation not only relates to the decomposition of oil, food and pharmaceutics but also to our living system, as it is related to oxidative stress and the death of cells by ferroptosis. Surprisingly, the fundamental mechanism underlying all of these materials' reactions with O2 is a radical-chain reaction with the well-known initiation, propagation, and termination stages [1]. Antioxidants play a fundamental role in the protection against the harmful effects of autoxidation. They act by trapping alkylperoxyl radicals (ROO•) that propagate the oxidative chain. The hydroperoxyl radical (HOO•) has been recently discovered as a significant player in modulating antioxidant activity in biosystems. The hydroperoxyl radical can regenerate antioxidants extending the duration of their activity, in particular for α-tocopherol (α-TOH) [2], the most potent form of vitamin E. Herein, we report that γ-terpinene, an essential oil component widely present in cardamom and other natural sources, has a remarkable antioxidant effect on the autoxidation of model membranes, represented by liposomes containing polyunsaturated phospholipids (from egg-yolk phosphatidylcholine). The mechanism of the antioxidant effect was clarified by performing theoretical calculation on the radical species originating form γ-terpinene oxidation. We found that oxidation of γ-terpinene affords HOO• radicals that, being hydrophilic radicals, exit the liposomes and block the oxidative chain. We anticipate that our findings will be of great significance in explaining the protective effects of essential oils in degenerative diseases because autoxidation plays a fundamental role in many pathologies.



Reference:
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[2] Poon J F , Zilka O , Pratt D A .Potent Ferroptosis Inhibitors Can Catalyze the Cross-Dismutation of Phospholipid-Derived Peroxyl Radicals and Hydroperoxyl Radicals[J]. Journal of the American Chemical Society, 2020.

POS68

Potent Anti-Tyrosinase Activity of Butein and Homobutein Probed by Computational and Kinetic Studies

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Melanin biosynthesis is regulated by enzyme Tyrosinase which is highly conserved in various organisms, including humans, plants, and animals. Tyrosinase is mainly involved in two distinct reactions, the monophenolase, which is the o-hydroxylation of a monophenol, then the diphenolase that converts an o-diphenol to the corresponding o-quinone. After that, o-quinone will undergo several spontaneous reactions to eventually form melanic pigments [1-3]. The goal of our research is the study of reversible enzyme inhibitors that would reduce the rate of the enzyme-catalyzed melanin production, focusing on inhibition kinetics and mechanism. Owing to the key role of melanin in shin pigmentation and food degradation, such compounds would have potential applications as food preservatives and skin depigmenting agents in dermatology [1].

Natural chalcones are a promising class of tyrosinase inhibitors [2], and current investigation focuses on Butein and Homobutein, as representative members found in different botanical sources [3]. By combined UV-Vis spectroscopy, fluorescence spectroscopy and oximetry kinetic studies [1], our data indicate for homobutein a potent mixed-type inhibition with prevalent of competitive behavior ($K_i \sim 2.5\ \mu$M) both toward monophenolase and diphenolase reactions [3]. Instead, butein showed nearly competitive inhibition only toward diphenolase reaction (substrate: L-dopa), while it was uncompetitive when the substrate was L-tyrosine (monophenolase reaction) [3]. Both chalcones outperformed reference Kojic acid. To rationalize their behavior, we turned to molecular docking computations, using Autodock Vina and Autodock-4 suites. We found the inhibitors' binding active site in the enzyme, and the best binding conformation with the enzyme for both inhibitors, which was compared to the best binding mode for native substrates, so to rationalize the inhibition. Two-ligand docking computations and the different binding interaction of butein and homobutein with the active-side aminoacid residues allowed to account for kinetic results. Overall, our study demonstrates and rationalizes the excellent anti-tyrosinase activity of butein and homobutein, highlighting their potential for target applications in food safety and in biomedical research [3].

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POS69

Researcher mental health and wellbeing within academia: the ReMO COST Action

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[5] COST Action CA19117 Researcher Mental Health Observatory

The ReMO COST Action CA19117 focuses on wellbeing and mental health within academia, a theme of strategic importance for the European Research Area.

ReMO involves a growing network of stakeholders from all levels of the research community, who work together to identify which practices and actions are effective at creating research environments that foster mental health and well-being, reduce mental health stigma, and empower researchers when it comes to well-being in their workplace.

Here we present the ReMO COST Action, its aim and objectives on assessing how the mental health and well-being of researchers can best be nourished and sustained through actions and initiatives at the policy, institutional, community and individual levels.

ReMO
Researcher Mental
Health Observatory

Gábor Kismihók. (2022, maggio 25). Researcher Mental Well-being. Zenodo. https://doi.org/10.5281/zenodo.6580384

Sponsors talks

SP01 – Giuseppe Tagliapietra (Merck)

SP02 – Mykola Borzenkov (Olon)

SP03 – Manuela Vacatello (Merck)

SP04 – (Eni)

SP01

Merck Life Science: Who We Are and What We Do

Gianluca Tagliapietra

Senior Vice President Commercial EMEA, Merck Life Science, Italy
E-mail: gianluca.tagliapietra@merckgroup.com

As a vibrant science and technology company, we believe in science as a force for good. More than 64,000 colleagues around the world are driven by a common aspiration: Advancing human progress. That's what we're committed to every day – across all of Merck. Our advanced treatment solutions and innovative technology are life-changing, influencing how we tackle major illnesses and integral to creating a better tomorrow. From cancer therapies and laboratory tools to smartphones, science and technology touch our lives. Our Life Science business accelerates access to health for people everywhere.

Before researchers can make scientific breakthroughs, they must have access to state-of-the-art tools, services, and expertise in order to perform experiments and engineer new products. That's where we come in. We offer one of the broadest portfolios in the industry for scientists and our presence extends well beyond the labs as our innovations touch individuals around the world. Together, we impact life and health with science.

SP02

Talent building program @OLON SpA

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Olon Group [1] is a global leader in the development and production of active pharmaceutical ingredients for CDMO and Generics, a reliable and preferential partner to the pharmaceutical, biotech, and specialty ingredients markets. With a 2022's turnover of 610 Mio$, OLON supplies 300 APIs for the Generic market.

Thanks to all the 2.300 employees, and to highly qualified R&D team – more than 300 people – OLON can offer complete integrated packages and services to support the full development of APIs based on strong knowledge in both Chemical and Biological process, all of them under a full cGMP and regulatory coverage – holder of about 160 active US DMFs and 79 granted CoS.

Headquartered in Rodano (Milan, Italy), OLON has 11 manufacturing facilities - 8 located in Italy, 1 in Spain, 1 in USA and 1 in India, designed in compliance with the strictest international requirements, and 3 branch offices in Hamburg (Germany), Florham Park NJ (USA) and Shanghai (China).

Talent building program will be presented within R&D careers.

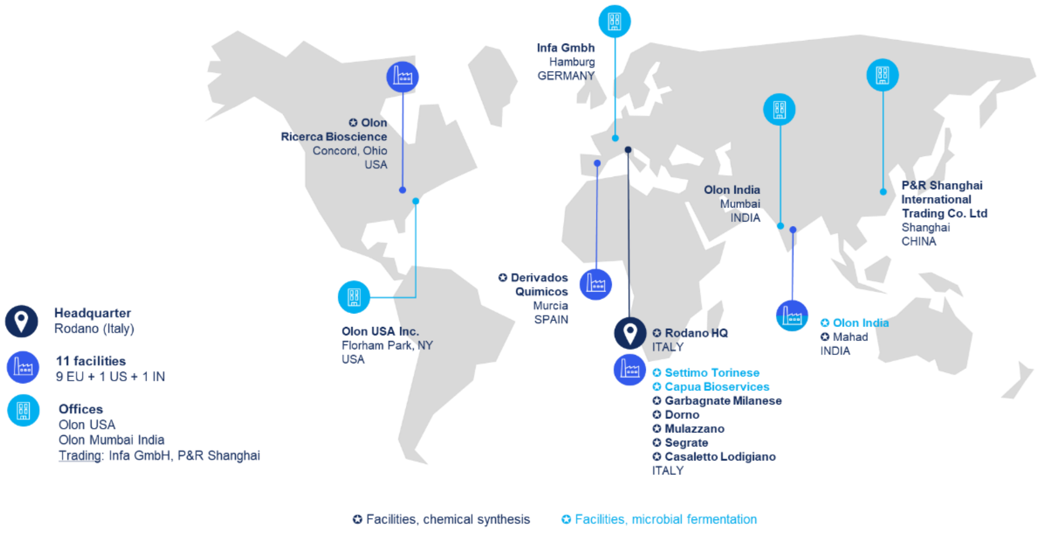

Figure 1: OLON facilities.

[1] www.olonspa.com

SP03

Merck Materials Science - Advanced Materials for Energy Storage

Manuela Vacatello

Scientific Saless Specialist for Chemistry and Analytical at Merck Life Science
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Merck KGaA Materials Science has made significant progress in the development of battery materials to enhance research in the energy storage field, addressing key challenges in battery performance.

In recent years we have continued our focus on improving battery energy density and cycle life stability through the introduction of novel materials and processes to enhance battery performance.

We collaborate closely with our academic partners to explore and design various materials for traditional and emerging battery chemistries such as fast charging and high energy density composites.

In this talk we will cover our recent successes in developing composite electrodes, which demonstrate increased energy density and stability across a range of devices including those manufactured through 3D printing.

We will also be highlighting preliminary results from our ongoing efforts on solid-state electrolytes and the development of more sustainable alternatives to commonly used battery materials.

SP04

List of participants

Name	Surname	Affiliation
Clelia	Aimone	Università degli studi di Torino
Giorgia	Albonetti	Università degli studi di Ferrara
Laura	Alessandroni	Università degli studi di Camerino
Stefano	Andolina	Università degli studi di Milano
Simona	Aprile	Università degli studi di Ferrara
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