Società Chimica Italiana
Sezione Puglia

Società Chimica Italiana
Gruppo Giovani

UNIVERSITÀ DEGLI STUDI DI BARI ALDO MORO
DIPARTIMENTO DI CHIMICA

Politecnico di Bari

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CHIMICA sotto l'albero

EDIZIONE 2024

INNOVATION FOR A GREEN, HEALTHY, AND DIGITAL WORLD

book of abstract

Book of Abstracts

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Edited by Mariachiara Bianco, Giovanni Ventura,
Cosima Damiana Calvano, Antonio Monopoli

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Awards

Best oral presentation

OR 41 - *Nanocellulose-based additives for paper wet strength: the interactions of chemically-modified nanofibers with commercial polyamidoamines*. Elisa FAGGIOLI – UniMI

Best flash presentations

FL 06 - *Integrating epoxidation and high-resolution mass spectrometry to unravel the complex profile of Boswellic acids in Boswellia serrata Gum Resin Extract.* Andrea CASTELLANETA – UniBA

FL 07 - *Development of a chromatography free method based on DART-Triple Quadrupole mass spectrometry for targeting safflower and turmeric as adulterants in saffron.*
Anna LUPARELLI – Cnr - ISPA

Best Poster presentations

P11 - *Advancing sensor technology: real-world applications of MIP-based sensors in Green Analytical Chemistry*. Marco COSTA – UniSalento DiSTeBA

P46 - *Cellulose-based nanostructured aerogels for leachate decontamination: towards sustainable phosphorus recovery from sewage sludge ash* - Laura RIVA – PoliMi

Awards sponsored by:

sustainable chemistry

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Premio per dottorandi

Il Corso di Dottorato in **Scienze Chimiche e Molecolari** dell'Università di Bari ha premiato con un attestato di merito Stefano SPERANZA per la flash communication intitolata *Chemical Interaction of Monoethanolamine (MEA) with Cooked Soil: A Step Towards the Reformulation of Home Care Products* (FL 24).

Il corso di dottorato di ricerca **Scienze del Farmaco** ha premiato con un attestato di merito Defne ŞERBETCI per l'oral communication intitolata *Synthesis of Aza-S(VI) Fluorides and Primary Sulfonimidamides from Sulfinylamines* (OR 03).

Il corso di dottorato industriale in **Tecnologie sostenibili per lo sviluppo industriale di medicinali e diagnostici (TeSSMeD)** ha premiato Gabriella Rosanna MUSILLO con un attestato di merito per la flash communication intitolata *Development of fluorescent ligands: greener and safer tools useful to drug discovery* (FL 13).

SCI fellowships:

Winners of Divisione di Chimica Analitica:

Federico GIROLAMETTI – UNIVPM DISVA P 20- *Heavy metals and metalloids in blackspotted smooth-hound sharks (Mustelus punctulatus) from the Southern Adriatic: contamination and dietary safety*

Sara PALMIERI – UniTE -OR 18 - *Phytocannabinoids profile in Cannabis sativa L. samples by means to LC-MRM/IDA/EPI analysis*

Winners of Divisione di Chimica Farmaceutica:

Giovanni GRAZIANO - UniBA OR 24- *AID-CARE: Artificial Intelligence-aided Design of CAnnabinoid REceptor subtype 2 (CB2R) Multitarget ligands: a new strategy for the treatment of inflammation*

Francesco MASTROPASQUA - UniBA OR 22- *Development of PET radiotracers for CNS diseases*

Morena MICIACCIA - UniBA OR 58- *Therapeutic Challenges in Pediatric Diffuse Intrinsic Pontine Glioma: Insights into the Structural Evolution of Human Protease ClpP Activators*

Viviana MITAROTONDA - UniBO -OR 26- *Development of Proteolysis Targeting Chimeras (PROTACs) and small molecule inhibitors for targeting neuroinflammation*

Daniele VITONE - UniBA -OR 60- *Pharmacokinetic Profiling and a Formulation Study on the FPR2 Agonist MR-39, a New Therapeutic Option for Autism Spectrum Disorder*

Winners of Divisione di Chimica Fisica:

Domenico CIGNOLO-UniBA – OR 06 - *Nanoengineered chitosan-based sponges for water remediation*

Dario LACALAMITA - UniBA – OR 09 - *Biohybrid Photocathode with Biobased Polymers for Green Hydrogen Production*

Rita MASTROGIACOMO-UniBA – OR 54 - *Large Pores Mesoporous Silica-Based Nanostructures and Nanostructured Lipid Carriers as Promising Nanotools for Gene Transfection in Cancer Immunotherapy*

Umberto MATTIA-UniBA – P 34 - *Engineering ceria nanoparticles to improve the performance of biohybrid microbial photoelectrodes*

Winners of Divisione di Chimica Organica:

Matteo Renato MARTINA- UniBA OR 02 - *Infrared light assisted arylation reactions catalysed by transition metal-based materials from electronic waste*

Davide MESTO- UniBA FL 25 - *From lignocellulosic biomasses to advanced biopolymers in just one step*

Stefano NEJROTTI – ISSMC-CNR OR 10 - *Enabling high proton conductivity in a fluorine-free protic ionic liquid through rational design of its constituents*

Carola RICCIARDELLI – UniBA FL 20 - *Silk Fibroin as a bioinspired organocatalyst for Michael addition reactions*

Cesar VICENTE-GARCIA – UniBA FL 11 - *Diatom Microrobots as effective and biodegradable agents against water-borne pollution*

Winners of Divisione di Chimica Industriale:

Stefano SAVINO – UniBA - OR 04 *Tunable Copper based slag catalyst for the production of energy vectors*

Antonio Cosimo Pio TRIMBOLI – UniRC – FL 18 - *Chemical Recycling of Waste Polyolefins via Catalytic Hydroconversion*

Winners of Divisione di Elettrochimica:

Francesco PANICO – UniMI – OR 45 - *Timeless Questions and Modern Challenges: Exploring the Origin of Life and Electrochemical CO_2 Reduction*

Winners of Divisione di Spettrometria di Massa:

Andrea CASTELLANETA – UniBA FL 06 - *Integrating epoxidation and high-resolution mass spectrometry to unravel the complex profile of Boswellic acids in Boswellia serrata Gum Resin Extract*

Ludovica Sofia GUADALUPI - UniBA OR 15 - *Could proteins be the secret to natural rubber's high-performance properties?*

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Thursday, december 19 Plenary 1- Sala Videoconferenze

08:15	Registration
09:00	Welcome and opening ceremony Presidente SCI Puglia - Antonio MONOPOLI Coordinatore SCI Giovani - Marta DA PIAN Presidente Nazionale SCI e delegato alla ricerca UNIBA – Gianluca Maria FARINOLA Presidentessa EuChemS– Angela AGOSTIANO Delegato del rettore POLIBA – Vito GALLO
	Chairs: Renzo Luisi, Piero Mastrorilli
09:30	**PL 01** – Combining Virtual Reality, Intelligent AI Avatars, 3D Printing and Low-cost Electronics: Global Interconnected Digital Laboratories Stephen HILTON- UCL School of Pharmacy

Thursday, 19 – PARALLEL Session 1-Sala Videoconferenze

	Chairs: Renzo Luisi, Piero Mastrorilli
10:00	**OR 01** - Synthesis of fluoroamides, acylfluorides and aminoamides through a divergent self-deoxyfluorination of bromodifluoromethyl alcohols in batch and mechanochemical conditions Giulia DE SANTIS-UniBA
10:15	**OR 02** - Infrared light assisted arylation reactions catalysed by transition metal-based materials from electronic waste Matteo Renato MARTINA - UniBA
10:30	**OR 03** - Synthesis of Aza-S(VI) Fluorides and Primary Sulfonimidamides from Sulfinylamines Defne ŞERBETCI- UniBA
10:45	**OR 04** - Tunable Copper based slag catalyst for the production of energy vectors Stefano SAVINO - UniBA
11:00	**OR 05** - Green synthesis of 2-L ferrihydrite supported on steel slags as catalyst for the reduction of nitroarenes Francesca DEROBERTIS - PoliBA

Thurday, 19 – PARALLEL Session 2- Sala Videoconferenze

	Chairs: Marta Da Pian, Emilia Paone
11:45	**FL 01** - Photocatalytically enabled umpolung for the synthesis of hydroxyalkylkated and fluoroalkylated motifs Yuri GELATO-UniBA
11:50	**FL 02** - A second life for e-waste: a catalyst from discarded capacitors active in the reduction of nitroarenes to anilines Alessia IENNACO-PoliBA
11:55	**OR 06** - Nanoengineered chitosan-based sponges for water remediation Domenico CIGNOLO - UniBA
12:10	**OR 07** - Comparison between thermal and plasma-enhanced Atomic Layer Deposition of ZnO on fullerene powder for photocatalytic dye removal Regina DEL SOLE -UniBA
12:25	**OR 08** - The seaweed Chaetomorpha linum (Chlorophyta, Cladophorales) as a bioremediator of microplastics Elisa QUARTA- IRSA, CNR, UniPA
12:40	**FL 03** - Study of eco-sustainable methods for reducing the organic fraction responsible for Chemical Oxygen Demand (COD) in wastewater from industrial plants Riccardo CICIRIELLO - UniBA
12:45	**FL 04** - Livestockfarm WasteWater (LWW) treatment through an advanced approach: the application of electrochemical oxidation Simona GALOPPO - University of Campania "Luigi Vanvitelli"
12:50	**OR 09** - Biohybrid Photocathode with Biobased Polymers for Green Hydrogen Production Dario LACALAMITA- UniBA
13:05	**OR 10 -** Enabling high proton conductivity in a fluorine-free protic ionic liquid through rational design of its constituents Stefano NEJROTTI - ISSMC CNR
13:20	**OR 11 -** Thin layer bismuth vanadate photoanodes for photoelectrochemical water oxidation Alberto MAGLIOCCO - UniFE
13:35	**Light Lunch & Poster Session (P01-P26)**

Thurday, 19 – PARALLEL Session 1- Sala Lettura

	Chairs: Cosima Damiana Calvano, Linda Monaci
10:00	**OR 12** - Aerosol assisted atmospheric pressure plasma deposition of quercetin containing coatings for food packaging application Angelica Maria LANZA-UniBA
10:15	**FL 05** - Green solvents as an alternative, sustainable practice for the recovery of phenolic compounds in grape pomace Vincenzo ROSELLI - UniBA
10:20	**FL 06**- Integrating epoxidation and high-resolution mass spectrometry to unravel the complex profile of Boswellic acids in *Boswellia* serrata Gum Resin Extract Andrea CASTELLANETA - UniBA
10:25	**FL 07** - Development of a chromatography free method based on DART-Triple Quadrupole mass spectrometry for targeting safflower and turmeric as adulterants in saffron Anna LUPARELLI – Cnr - ISPA
10:30	**OR 13** - A RPLC-APCI-FTMS method to characterize and quantify phytosterols in Apulian Brassicaceae vegetable products Valeria CINQUEPALMI - UniBA
10:45	**OR 14-** Determination of 2-dodecylcyclobutanone and 2-tetradecylciclobutanone in X ray irradiated whole eggs: a green method Andrea CHIAPPINELLI- IZS-Foggia
11:00	**OR 15** - Could proteins be the secret to natural rubber's high-performance properties? Ludovica Sofia GUADALUPI- UniBA
11:15	**Coffee BREAK**

Thurday, 19 – PARALLEL Session 2- Sala Lettura

	Chairs: Federico Fanti, Marco Iammarino
11:45	**FL 08** - Investigating the effect of different cooking treatments on the formation of polycyclic aromatic hydrocarbons in meats by means of GC-MS/MS Mariateresa INGEGNO- IZS-Foggia
11:50	**OR 16** - Unlocking Nature's Palette: Enhancing Green Extraction of Anthocyanins from Apulian Pigmented Wheat Landraces Davide CONIGLIO-UniBA
12:05	**OR 17** - Enhancing Hydroponic Farming with Vermitea: A Sustainable Alternative to Chemical Nutrient Solutions Sami ur REHMAN- UniSalento
12:20	**OR 18** - Phytocannabinoids profile in Cannabis sativa L. samples by means to LC-MRM/IDA/EPI analysis Sara PALMIERI -UniTE
12:35	**FL 09** - Separation and analysis of the cis- enantiomers of Cypermethrin based on QuEChERS and GC-MS/MS analysis Ines DELLA ROVERE- IZS-Foggia
12:40	**OR 19**- Exploring cheese whey permeate as raw material for the chemoenzymatic synthesis of bio-based emulsifiers Giorgia BALLABIO -UniMI
12:55	**FL 10**- Alkaline Phosphatase Inhibition on Gold Nanocoral Electrodes for the Ultrasensitive Detection of 2,4-Dichlorophenoxyacetic Angelo TRICASE -UniBA
13:00	**OR 20** - A Novel Approach to Radiochemical Determination of Ra, Th and U in Solids Michele NICOLINI IZS-Foggia
13:15	**OR 21 -** Polyphenols as Key Markers for Machine Learning-Based Olive Cultivar Classification Fabiola EUGELIO - UniTE
13:30	**FL 11 -** Diatom Microrobots as effective and biodegradable agents against water-borne pollution Cesar VICENTE-GARCIA - UniBA
13:35	**Light Lunch & Poster Session (P01-P26)**

Thursday, 19 –Plenary 2- Sala Videoconferenze

	Chairs: Giovanni Lentini, Antonio Monopoli
14:45	**SP 01** - Andriani Società Benefit: salute e benessere delle persone Maria Teresa BURDO e Rossella LABARBUTA- Andriani SpA
14:55	**SP 02** – Enzyme production by E.Coli fermentation at pilot scale: a case study Alberto DE RICCARDIS - Euroapi
15:05	**GS 01** –Intendere il progresso come un processo: gli archivi per la storia della chimica Guest Speaker: Federico BERRETTA - Roma La Sapienza

Thursday, 19 – PARALLEL Afternoon Session 1-Sala Videoconferenze

Chairs: Giovanni Lentini, Antonio Monopoli

15:30	**OR 22** - Development of PET radiotracers for CNS diseases – Francesco MASTROPASQUA - UniBA
15:45	**OR 23** - Comparative Analysis of Single Molecule Transistor (SiMoT) Technology and Ultrasensitive Immunoassay Array Technologies Mariapia CAPUTO- UniBA
16:00	**OR 24**- AID-CARE: Artificial Intelligence-aided Design of CAnnabinoid REceptor subtype 2 (CB2R) Multitarget ligands: a new strategy for the treatment of inflammation Giovanni GRAZIANO – UniBA
16:15	**OR 25-** Development of an electrochemical sensor for cardiac troponin T based on molecularly imprinted nanoparticles produced by solid-phase synthesis via epitope imprinting approach Francesco GAGLIANI- UniSalento
16:30	Coffee BREAK

Thursday, 19– PARALLEL Afternoon Session 2 Sala Videoconferenze

Chairs: Enza Lacivita, Angela Stefanachi

17:00	**OR 26 -** Development of Proteolysis Targeting Chimeras (PROTACs) and small molecule inhibitors for targeting neuroinflammation Viviana MITAROTONDA- UniBO
17:15	**OR 27** - Ultra-sensitive and rapid detection of SARS-CoV-2 subgenomic RNA using a single-molecule with a large transistor-SiMoT bioelectronic platform Francesca INTRANUOVO - UniBA
17:30	**FL 12** - Development of potent mitochondrial hClpP activators for cancer therapy through a process of structural simplification Domenico ARMENISE- UniBA
17:35	**FL 13** - Development of fluorescent ligands: greener and safer tools useful to drug discovery Gabriella Rosanna MUSILLO - UniBA
17:40	**FL 14** - Assessing the Antitumor Potential of Monofunctional Platinum(II)-Nucleoside Complexes: Synthesis, Characterization, and Cytotoxicity Studies of cis-[Pt(NH3)2(Guo/dGuo)X] (X = Cl, Br, I) Erika STEFANO - UniSalento
17:45	**OR 28** - 2- Aryloxymethylene-substituted scaffolds as privileged moieties for the design of new potential metal chelators in the multi-target therapy of Alzheimer's disease Rosalba LEUCI - UniBA
20:00	*Social dinner at Seconda Classe*

Thursday, 19 – PARALLEL Afternoon Session 1-Sala Lettura

Chairs: Enza Lacivita, Angela Stefanachi

15:30	**OR 29-**Next-Generation FPR2 Agonists: Leveraging Multicomponent Reactions to Improve Drug-Like Properties Fabio FRANCAVILLA- UniBA
15:45	**OR 30** - SIGMAP: an explainable artificial intelligence tool for SIGMA-1 receptor affinity Prediction Maria Cristina LOMUSCIO – UniBA
16:00	**OR 31**- Intelligent design of novel multi-target antibiotics against superbugs Anna Rita TONDO - UniBA
16:15	**OR 32-** Innovative Approach to FTIR Spectroscopy: Use of Artificial Intelligence for Quantitative Analysis of the Paleolithic Site at Riparo Mochi Alessia SANTIGLIA– UniMI

Thursday, 19 – PARALLEL Afternoon Session 2-Sala Lettura

Chairs: Antonio Monopoli, Rosaria Anna Picca

17:00	**OR 33** - Self-calibrated Laser Induced Breakdown Spectroscopy for in situ monitoring of Volcanic Ash. Aya TALEB - UniBA
17:15	**OR 34** - Analytical insights into action mechanisms of ZnO-based bioactive coatings by scanning electrochemical microscopy Margherita IZZI- UniBA
17:30	**OR 35** - NIR spectroscopic profiling of a progressive air purification system for indoor Cultural Heritage spaces Anna Laura TASSI - UniMI
17:45	**FL 15** - Composite electrodes for enhanced ozone-based water treatment: development and characterization of nanostructured titanium substrates Chiara FREZZA – UniRoma3
17:50	**FL 16** - Pectin/Gellan gum hydrogel films embedded with saffron by-products: a promising strategy for wound healing Francesco BUSTO- UniBA
17:55	**FL 17** - Advanced x-ray scattering techniques for structural characterization of antibacterial nanostructured biomaterials Erika MANICONE – UniBA-CNR
20:00	*Social dinner at Seconda Classe*

	Friday, 20 – Plenary 3-Sala videoconferenze
	Chairs: Renzo Luisi, Antonio Monopoli
09:00	**PL 02** – Precision Labeling of Small Molecules Joseph R. CLARK-University of Tennessee, Department of Chemistry, Knoxville, USA
09:30	**SP 03**- Orbitrap Exploris GC: a complementary technique for metabolomics studies Paolo BENEDETTI-Thermo Scientific
09:40	**SP 04** – LabService – Soluzioni innovative per applicazioni in flow-chemistry Antonio FORNARO - Lab Service Analytica S.R.L.
	Friday, 20– PARALLEL Morning Session 1 Sala videoconferenze
	Chairs: Renzo Luisi, Emilia Paone
10:00	**OR 36** - Radical Mediated Decarboxylation of Amino Acids via Photochemical Carbonyl Sulfide (COS) Elimination Lorenzo DI SIMO- Trinity College-UniPI
10:15	**FL 18** - Chemical Recycling of Waste Polyolefins via Catalytic Hydroconversion Antonio Cosimo TRIMBOLI- UniRC
10:20	**FL 19** - Reactive behaviour of Platinum(II) salts with ethylenediamine in sustainable water-choline chloride based deep eutectic solvents mixtures Nicola GAROFALO- UniSalento
10:25	**FL 20** - Silk Fibroin as a bioinspired organocatalyst for Michael addition reactions Carola RICCIARDELLI-UniBA
10:30	**OR 38** Future-proofing historic carbonatic and pyroclastic rocks via application of ammonium hydrogen phenylphosphonate Simone MURGIA- UniCA
11:00	Coffee BREAK
	Friday, 20– PARALLEL Morning Session 1 Sala lettura
	Chairs: Rosalia Zianni, Federico Fanti
10:00	**FL 21** - PLA@Croconaine matrix as a photothermal layer: photophysical and thermal investigations Maria MONTRONE- UniBA
10:05	**FL 22** Natural urease inhibitors from lignocellulose - Vanessa SPADAVECCHIA- UniBO
10:10	**OR 37** Green transition in food authentication: G-score driving method development Antonella LAMONACA - Cnr-ISPA
10:25	**OR 39** Aptamer-Enhanced Electrochemical Biosensor for the Detection of *Listeria monocytogenes* Giuseppe LAMBERTO- UniSalento
11:00	Coffee BREAK
	Friday, 20– Plenary 4-Sala Videoconferenze
	Chairs: Livia Giotta, Gian Paolo Suranna
11:45	**SP 05** –NexION 2200 & 5000. L'interfaccia di nuova generazione Paolo SESSA, Perkin Elmer - Field Application Specialist Inorganic
11:55	**PL 03** – Luisa DE MARCO – CNR NANOTECH - Energy Storage in Sustainable Hybrid Nanostructured Systems
	Friday, 20– PARALLEL Morning Session 2- Sala Videoconferenze
	Chairs: Livia Giotta, Gian Paolo Suranna
12:30	**FL 23** An initial assessment of Deep Eutectic Solvents on bacterial photosynthesis Claudia ZONNO- UniPG-UniBA
12:35	**FL 24** Chemical Interaction of Monoethanolamine (MEA) with Cooked Soil: A Step Towards the Reformulation of Home Care Products Stefano SPERANZA-UniBA
12:40	**FL 25**- From lignocellulosic biomasses to advanced biopolymers in just one step Davide MESTO- UniBA
12:45	**OR 40** Thermochromic Polymeric Composite Based on 2D Hybrid Organic–Inorganic Perovskite Bruno SIMONE-CNR-Nanotec
13:00	**OR 41** Nanocellulose-based additives for paper wet strength: the interactions of chemically-modified nanofibers with commercial polyamidoamines Elisa Giovanna FAGGIOLI-UniMI
13:15	**OR 42** Dual-functionality starch film with conductive and antibacterial properties enabled by dicationic ionic liquid plasticizers for flexible electronics Susanna ROMANO-UniRoma3
13:30	**OR 43 -** Barrier performances of cellulose nanofibers-based coating agents in paper industry Arianna DE SANTIS-PoliMI
13:45	Light Lunch & Poster Session (P27-P52)

Friday, 20– PARALLEL Morning Session 2- Sala Lettura

Chairs: Marta Da Pian, Maria Michela Dell'Anna

12:30	**OR 44** Versatile vapor-phase MIP deposition on nanostructured PSiO2 optical transducer for label-free quercetin sensing Muhammad Ibrar ASIF- UniSalento
12:45	**OR 45** Timeless Questions and Modern Challenges: Exploring the Origin of Life and Electrochemical CO_2 Reduction Francesco PANICO- UniMI
13:00	**OR 46** Unveiling the Effect of Mechanical Exfoliation and Surfactant Intercalation on Multi-layered Graphene Conductive Inks Michele CATACCHIO- UniBA
13:15	**OR 47** Effect of chemical structure and electrolyte on the electrochemical energy storage properties of quinone derivatives Martina SCARAMUZZO- CNR-Nanotec
13:30	**OR 48 -** Superabsorbent Hydrogels Based on Pectin and Succinic Anhydride Stefano LIOTINO- UniBA
13:45	**Light Lunch & Poster Session (P27-P53)**

Friday, 20 – PARALLEL Afternoon Session Sala videoconferenze

Chairs: Rosaria Anna Picca, Maurizio Quinto

15:00	**OR 49-** Carbon-Based Materials and Microfluidic Platforms for Neural Tissue Regeneration: Towards Integrated In Vitro Models for Brain Repair Antonella IAIA-CNR-Nanotec
15:15	**OR 50**- Luminescent Zero-Dimensional Inorganic Perovskite-Photocurable Resin for Scintillator Mario CALORA-CNR-Nanotec
15:30	**OR 51** - Camphorsulfonic-Salified Chitosan Allowing MACl-Free Stabilization of Pure FAPbI3 α-Phase via Gravure Printing in Ambient Air Nadir VANNI-UniSalento
15:45	**OR 52** - Plasma-treated thermoresponsive hydrogels as RONS delivery systems for colorectal cancer therapy Angela PIGNATELLI-CNR-Nanotec
16:00	**OR 53** - Novel Hybrid Nanocomposites based on Au Nanoparticles decorating Viticulture Biomass-derived Graphene Oxide and Soot Carbon Waste Nanoparticles Stefano DICORATO-Nanotec
16:15	**OR 54 -** Large Pores Mesoporous Silica-Based Nanostructures and Nanostructured Lipid Carriers as Promising Nanotools for Gene Transfection in Cancer Immunotherapy Rita MASTROGIACOMO- UniBA
16:30	**OR 55** - Versatile Conductive Ink Formulations for Flexible, Wearable, and Edible Enzyme-Based Biosensors Verdiana MARCHIANO' – UniBA

Friday, 20 – PARALLEL Afternoon Session- Sala Lettura

Chairs: Cosima Damiana Calvano, Maria Grazia Perrone

15:00	**OR 56**- Evaluation of the Biological Properties of a Multifunctional Natural Supplement for Liver Protection Alexia BARBAROSSA – UniBA
15:15	**FL 26** Decoding Organic Binders in Art: Hydrogel Micro-Extraction and MALDI-MS for Non-Invasive Identification of Natural Gums Elena RIGANTE- UniBA
15:20	**FL 27-** Photonic Nanostructures from organic fluorophores and biosilica Vincenzo TEDESCHI- UniBA
15:25	**OR 57** - H2S releasing FPR2 agonists against neuroinflammation Leonardo BRUNETTI UniBA
15:40	**OR 58** - Therapeutic Challenges in Pediatric Diffuse Intrinsic Pontine Glioma: Insights into the Structural Evolution of Human Protease ClpP Activators Morena MICIACCIA- UniBA
15:55	**OR 59-** Rational optimization of the N-adamantyl-anthranil amide structural core for the development of new selective ligands for the Cannabinoid subtype 2 Receptor (CB2R) Annalisa FANIZZI- UniBA
16:10	**OR 60 -** Pharmacokinetic Profiling and a Formulation Study on the FPR2 Agonist MR-39, a New Therapeutic Option for Autism Spectrum Disorder Daniele VITONE- UniBA
16:25	**FL 28-** Development of P2X7 receptor antagonists for modulating immune response in neurodegenerative disorder with improved drug-like properties Angela SANTO - UniBA
16:30	**OR 61**- Development of ligands with high affinity for the pluripotent chaperon sigma1 (σ1) as potential anti-SARS-CoV-2 agents. Anna Teresa LISI - UniBA

Awards ceremony, closing of the congress
Christmas greetings with Panettone & Spumante

Poster session Thursday, 19 DECEMBER (P01-P26)
P01 - Bottom-up proteomics for identifying and quantifying soybeans and mustard allergens in processed food matrices - Mariachiara BIANCO – UniBA
P02 - Electrochemical Impedance Spectroscopy Investigations on MnO_2-based Gas Diffusion Electrodes for Zinc-air batteries - Francesco BISCAGLIA – UniSalento CNR NANOTEC
P03 - Daunian Ceramics Under The Lens: A Multi-Technique Investigation To Uncover The Past- - Claudia BISCOTTI - UniBA
P04 - Self-powered wearable biosensor with stencil-printed carbon nanotube electrodes for monitoring sweat ethanol levels - Blanca Maria Iolanda CASSANO – UniBA
P05 - Choline acetate as a novel ionic liquid for Sonogashira cross-coupling reaction - Tommaso CASTIGLIA – UniBA
P06 - Identification of X-ray irradiated peanuts by DNA comet assay and HS-SPME/GC-MS analysis - Francesca CATANO – IZSPB
P07- Preliminary Study For The Development Of New Dual Agonists Of PPAR And FXR For The Treatment Of Metabolic Dysfunction-Associated Steatohepatitis (MASH) - Marco CERINI – UniBA
P08 - Edible Amperometric Biosensors for Intestinal Monitoring of Glucose Levels - Alessandra CIMINO – UniBA
P09 - Functionalized MALDI matrices for the analysis of low molecular weight compounds - Andrea CINNIRELLA – UniBA
P10 - Volatolomics based on HS-SPME/GC-MS and multivariate analysis for the characterization of volatiles in peels of prickly pear and pomegranate - Alessandra COMO – UniFg
P11 - Advancing sensor technology: real-world applications of MIP-based sensors in Green Analytical Chemistry - Marco COSTA – UniSalento DiSTeBA
P12 - Plasma-Based Modification of Tin Halide Perovskite Interfaces for Photovoltaic Applications - Sara COVELLA – UniBA
P13 - Tailoring the corrosion behaviour in body fluids of superplastically formed magnesium alloy resorbable implants by means of surface coatings - Angela CUSANNO – PoliBA DMMM
P14 - Characterization of atmospheric particulate matter by ATR-FTIR spectroscopy in the framework of TOX-IN-AIR project - Ylenia DE LUCA – UniSalento DiSTeBA
P15- Sustainable Mechanochemical Approach for Graphene-Based Pellet Production in Additive Manufacturing - Roberta DI MAIO – UniSalento CNR NANOTEC
P16 - On-demand bioresorbable opto-electronic sensors for in-vivo and in-situ monitoring of chemotherapeutic drugs and biomarkers - Tiziano DI GIULIO – UniSalento DiSTeBA
P17 - Novel molecularly imprinted polymers (MIPs) based on natural phenols combined with Au nanoparticles for sensing applications - Khadija EDDAHAOUI – UniSalento DiSTeBA
P18 - Electrosynthesis of Zinc Oxide-based nanoantimicrobials with Benzalkonium Chloride: Optimization and Analytical characterization - Alessandro FARANDA – UniBA
P19- Preliminary 1H-NMR characterization of stabilized grape pomace extracts - Miriana Carla FAZZI – UniSalento DiSTeBA
P20 - Heavy metals and metalloids in blackspotted smooth-hound sharks (Mustelus punctulatus) from the Southern Adriatic: contamination and dietary safety – Federico GIROLAMETTI – UNIVPM DISVA
P21 - 1-Oxa-2,6-diazaspiro[3.3]heptane as a New Potential Piperazine Bioisostere – Flow-Assisted Preparation and Derivatisation by Strain-Release of Azabicyclo[1.1.0]butanes - Elena GRAZIANO – UniBA
P22 - Spectroscopy-based metabolomics for early detection of Citrus Tristeza Virus infection Annamaria GRECO – PoliBA DICATECH
P23 - Lignin valorisation for biofuel and chemicals production - Peyman HAMIDIZADEH – PoliBA
P24 - Towards sustainable materials and chemicals: extraction and characterization of mucilage polysaccharides from Opuntia-ficus indica - Federica lACONETA – UniSalento DiSTeBA
P25 - Natural Deep Eutectic Solvents and Ultrasound-Assisted Extraction (NADEs-UAE): A Novel Approach for Polyphenol Extraction from Endemic Apulian Salicornia europaea L. - Francesco LIMONGELLI – UniBA
P26- Determination of volatile organic compounds (VOCs) in indoor work environments by solid phase microextraction-gas chromatography-mass spectrometry- Donatella NARDIELLO - UniFG

Poster session Friday, 20 DECEMBER (P27-P53)
P27- PK/PD of imipridone-based mitochondrial hClpP activators - Anselma LITURRI – UniBA
P28 - Advancing Tin-Based Perovskite Solar Cells: Interface Engineering with Chelating Agents for Enhanced Stability and Performance - Lucia MERCURIO – UniSalento CNR NANOTEC
P29 - In Vitro Validation of Cannabinoid Receptor Subtype 2 (CB2R) Selective Fluorescent Probes SM15 And VM7– Mariachiara MAMMONE – UniBA
P30 - Green Recovery of High Value-Added Products From Shrimp Wastes For A Sustainable Economy - Federica MANCARELLA – UniSalento DiSTeBA
P31 - Source Apportionment of Real-Time Ultrafine Particulate Matter in a Mediterranean Urban Center During the Summer - Antonio MANCO – UniSalento DiSTeBA
P32 - Synthesis of Aza-S(VI) Fluorides and Primary Sulfonimidamides from Sulfinylamines - Laura MARRAFFA – UniBA
P33 - Electrochemical and spectroscopical characterization of apta-sensor based on poly-L-Dopa modified gold electrodes - Laura MARTINA – UniSalento DiSTeBA
P34 - Engineering ceria nanoparticles to improve the performance of biohybrid microbial photoelectrodes - Umberto MATTIA – UniBA
P35 - Extraction and purification of antimicrobial peptides and their adsorption on mesoporous silica nanoparticles - Gaia Maria MELONI – UniCa
P36 - Nanostructured cathodes functionalized with redox molecules for energy storage- Giuseppe MIANULLI – UniSalento CNR NANOTEC
P37 - Structural Implications of Missense Point Mutations in SBDS: Insights from a combined SAXS/MD investigation - Vittoria NANNA – CNR Istituto di Cristallografia
P38 - Waste Treatment and Disposal Plant: evaluation of emission impact and air quality - Celeste NAPOLITANO – UNIVPM DISVA
P39 - LC-MS characterization of allergens released by innovative food packaging - Vito NETTIS – UniBA
P40 - In vitro bio-characterization of Mesoporous Silica Nanoparticles for controlled Deferoxamine delivery - Monica ONRUBIA – Universidad Rey Juan Carlos
P41 - Deep Eutectic Solvents for New Low Environmental Impact Methodologies for Polymer Waste Transformation - Andrea Nicola PAPARELLA – UniBA
P42 - Nature-Inspired Design Of New Anti-Alzheimer's Multi-Target Drugs: The NInFA project - Marco PAPARELLA – UniBA
P43 - Lipidomic analysis of edible insects by LC-MS - Michele PELLEGRINO – UniBA
P44 - Oxidative Potential of Particulate Matter: new multi-sample analysis protocol - Serena POTÌ – UniSalento CNR ISAC
P45 - Design and synthesis of a bicyclic peptide analogue of the β-sheet domain of arc repressor - Eleonora PROCINO – Ud'A Chieti Pescara
P46 - Cellulose-based nanostructured aerogels for leachate decontamination: towards sustainable phosphorus recovery from sewage sludge ash - Laura RIVA – PoliMi
P47- Advanced biosensors for early detection of clinically relevant biomarkers - Lucia SARCINA – UniBA
P48 - Development of Synthetic Polymers as Sustainable Release Agents – Alessia SCARPIELLO – PoliBA DICATECH
P49 - Ag_3PO_4-based nanostructures for antimicrobial coatings - Claudio STUCCHI – UniBA
P50 - Quantitative and Non-Targeted NMR Approaches in Metrological Traceability – Maria TRISOLINI – PoliBA DICATECH
P51 - LC-MS Profiling of Bioactive Compounds from Agricultural By-products for Pharmaceutical and Biofuel Applications – Giovanni VENTURA – UniBA
P52 - Reshaping Ritter Reaction in Deep Eutectic Solvents: Sustainable Synthesis of Amides – Arfa YOUSAF – UniBA
P53 - Natural urease inhibitors from lignocellulose - Vanessa SPADAVECCHIA- UniBO

Summary

Flash Presentations

Poster Presentations

Invited Lectures

Combining Virtual Reality, Intelligent AI Avatars, 3D Printing and Low cost Electronics: Global Interconnected Digital Laboratories

Stephen Hilton

UCL School of Pharmacy

Advancements in Virtual Reality (VR), artificial intelligence (AI), and 3D printing are revolutionising how scientific research and collaboration are conducted. This talk explores the concept of Global Interconnected Digital Laboratories, where cutting-edge technologies combine to solve challenges in global collaboration, training standardization, and resource accessibility across multiple time zones and languages. We present our experience and vision of Digital Virtual Centres powered by intelligent conversational AI avatars, enabling seamless 24/7 global collaboration across time zones. These centres utilise VR-based digitisation of equipment and environments, allowing for real-time interaction and training while minimising costs and carbon footprints. AI avatars act as co-pilots, providing personalised guidance in experimental setups, health and safety, and chemical planning, enhancing efficiency and safety.

Incorporating 3D printing and low-cost electronics, these centres enable access to advanced scientific equipment. Customizable VR workflows integrate with continuous flow systems, allowing for global telemetry, data visualization, and real-time experimentation. The talk will showcase key uses in our laboratories, including VR-based HPLC training, digital twin integration, and scalable VR outreach for STEM education. By reimagining laboratory infrastructures, we aim to build a collaborative, accessible, and sustainable future for science.

Precision Labeling of Small Molecules

Joseph R. Clark

University of Tennessee, Department of Chemistry, Knoxville, USA

Despite the tremendous utility that precisely deuterated small molecules have in chemical research and the development of new medicines, methods to selectively incorporate this isotopic label into molecular scaffolds are lagging. Not only is highly selective deuterium labelling challenging, but spectroscopic techniques to support advances in selective labelling reaction discovery are sometimes inadequate. Catalytic transfer deuteration and hydrodeuteration reactions are uniquely equipped to precisely install deuterium into small molecules [1].

New copper-catalyzed reactions for the selective transfer deuteration and hydrodeuteration of alkene and alkyne-containing small molecules will be discussed along with novel spectroscopic techniques for the analysis of isotopic products [2-5].

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Energy Storage in Sustainable Hybrid Nanostructured Systems

Luisa De Marco

Institute of Nanotechnology of National Research Council – CNR NANOTEC –
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Energy storage devices are essential for the clean energy transition, enabling the use of renewable energy and supporting electric mobility. While Lithium-Ion Batteries (LIBs) offer several desirable features, such as high efficiency and long lifetimes[1], the rapid growth of their market has raised concerns about the availability of raw materials. Current projections suggest a potential shortage within the next decade[2].

To support the green transition, the development of innovative battery technologies with a low environmental footprint and sustainable materials is crucial. Organic redox materials are among the most promising candidates, as they can be sustainably produced, either from biomass or through green synthetic processes[3].

This research aims to develop new environmentally friendly systems inspired by organic molecules used in the chemistry of life for the storage of chemical energy and its transformation in electrical energy. The goal is to revolutionize traditional battery electrode design by introducing an innovative architecture that combines organic redox molecules with carefully tailored nanostructures.

This technology has the potential to establish a new paradigm for sustainable electrochemical energy storage, offering exceptional versatility in both electrode materials and electrolytes.

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Guest Speaker

Intendere il progresso come un processo: gli archivi per la storia della chimica

Federico Berretta

Sapienza - Università di Roma

Pare che il celebre fisico Richard Feynman una volta si sia espresso con una iconica battuta:" La filosofia della scienza è utile agli scienziati più o meno quanto l'ornitologia lo è agli uccelli". È lecito presumere che la critica non troppo velata si possa estendere a tutte quelle discipline che, pur interessandosi dell'attività dello scienziato, non abbiano un repentino e valutabile impatto sul suo lavoro: lo studio e la gestione degli archivi della chimica parrebbe essere una di queste. Ma è davvero così? Attraverso questo contributo si cercherà di dimostrare come l'archivistica, seppur non indispensabile alla chimica, potrebbe essere quantomeno auspicabile, ragionando sulle opportunità economiche, storiche e identitarie che la disciplina ha da offrire. Nel farlo si passeranno in rassegna le carte di alcuni dei più famosi chimici della storia italiana, quelle della Società Chimica Italiana, del CNR, delle università e di altri enti che trainarono la ricerca scientifica; documenti nei quali la componente scientifica si amalgama con quella politica, sociale e umana restituendo uno spaccato su un mondo che non esiste più, ma che non manca di influenzare ancora fortemente il nostro modo di vedere le cose e di affrontare il presente.

Oral Presentation

Synthesis of fluoroamides, acylfluorides and aminoamides through a divergent self-deoxyfluorination of bromodifluoromethyl alcohols in batch and mechanochemical conditions

Giulia De Santis, Marco Colella, Mauro Spennacchio, Michael Andresini, Renzo Luisi, Leonardo Degennaro

Dipartimento di Farmacia, Università degli Studi di Bari Aldo Moro, 70126 Bari, Italy

Organofluorine compounds hold an increasingly central role in the scientific landscape, involving not only drug synthesis but also the chemical production of materials. The introduction of fluorine atoms into organic molecules often originates radical changes into their chemical and biological properties. Therefore, an increasing number of new synthetic strategies involve fluorine integration into pharmaceuticals, agrochemicals, and advanced materials[1]. In the last few months, in my research group, we have developed an innovative synthetic strategy that involves a pre-installed halodifluoromethyl unit that can be used as a fluoromethyl or fluorocarbonyl source through multiple cleavage involving both C–F and C–X bonds (deconstructive mode)[2]. In particular, we were able to obtain a diverse range of valuable N-containing compounds such as a-fluoroamides, a-aminoacylfluorides and a-aminoamides using bromodifluoromethyl group as a C1 and F1 synthon, under basic conditions and in the presence of amines (Figure 1). Our synthetic approach offers a promising alternative to traditional methods for producing fluorinated compounds, which are often complex, require high temperatures, or involve environmentally harmful solvents and reagents. Additionally, our platform is adaptable to various technologies, including mechanochemistry[3]. This emerging technique provides a more sustainable and environmentally friendly alternative to conventional batch synthesis and is becoming increasingly significant in the organic chemistry panorama.

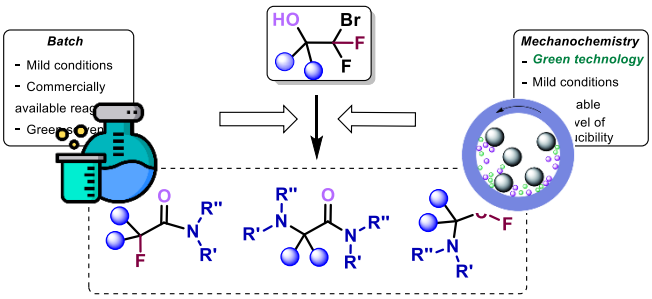

Figure 1: Synthesis of fluorinated molecules both in batch and in mechanical conditions

Acknowledgements: We thank the European Commission – Horizon Europe Framework, project SusPharma grant agreement No 101057430 for financial support and the Italian MUR financial support of PRIN 2022 code number n. 20228W9TBL.

Keywords: Fluorine, Green, Mechanochemistry.

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Infrared light assisted arylation reactions catalysed by transition metal-based materials from electronic waste

Matteo Renato Martina, Gianluca Maria Farinola, Pietro Cotugno, Roberta Ragni

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Synthetic protocols based on the use of non-conventional heating methods and catalytically active materials recycled from waste are gaining great attention in view of their huge potential to face the issues of depletion of raw materials and environmental impact in organic synthesis. In this framework, heating methods based on irradiation by infrared (IR) light allow performing reactions in shorter times and lower energy consumption versus conventional thermal heating, as well as with higher reaction yields and better chemoselectivity[1]. In addition, among the extremely high variety of waste produced worldwide, electronic waste can be regarded as a profitable source of transition metals with well-known catalytic activity in organic reactions. In particular, MultiLayer Ceramic Capacitors (MLCCs)[2] recovered from electronic components of end-of-life circuits and devices represent valuable sources of heterogeneous supported catalysts for a great variety of transition metal catalysed organic reactions. The combination of IR-assisted and MLCC-catalyzed synthetic protocols is expected to pave the way to innovative strategies still unexplored in the current scientific literature. On this ground, here we provide the first proofs of evidence of their great potential in the field of organic chemistry and materials science, exploring IR-light assisted and MLCC-catalyzed Buchwald-Hartwig reactions of a series of substituted indoles with aryl halides[3]. Comparison with thermal heating methods and more conventional organometallic catalysts also demonstrates the good performances of the new strategy investigated.

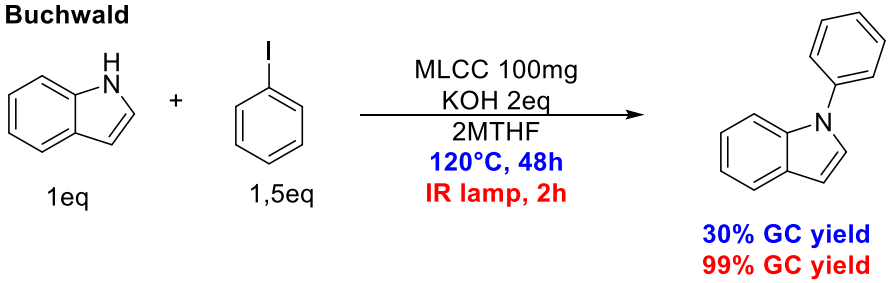

Figure 1: Buchwald reaction under Conventional Heating (blue) and under Infrared Irradiation (red)

Keywords: *Infrared-Light, E-waste, Buchwald reaction.*

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Synthesis of Aza-S(VI) Fluorides and Primary Sulfonimidamides from Sulfinylamines

Defne Şerbetçi, Michael Andresini, Laura Marraffa, Philipp Natho, Marco Colella, Leonardo Degennaro, Renzo Luisi

FLAME-Lab, Flow Chemistry and Microreactor Technology Laboratory, Department of Pharmacy – Drug Sciences, University of Bari, "A. Moro" Via E. Orabona 4, 70125 Bari, Italy

Hexavalent sulfur fluorides are strategic electrophilic reagents in organic synthesis enabling the linkage of S-O, S-N and S-C bonds[1]. While the preparation and use of sulfonyl fluorides have been widely explored, very little information about the synthesis and reactivity of sulfonyl fluoride aza-isosters, namely sulfonimidoyl fluorides and sulfondiimidoyl fluorides, is currently available[2,3]. Moreover, these compounds can be prepared through lengthy and time-consuming synthetic routes, that often require the generation of more reactive intermediates such as aza-S(VI) chlorides[4], or gaseous reagents[5]. Considering the great potential of such S(VI) derivatives in enabling the straightforward preparation of sulfur pharmacophores, here we present a fast one-pot synthesis of both sulfonimidoyl fluorides and sulfondiimidoyl fluorides starting from sulfinyl amines. The transformations proceed via nucleophilic addition of organometallic reagents to sulfinyl amines and sulfurdiimides[6,7], in turn prepared in situ from sulfinyl amines, followed by subsequent quenching with an electrophilic fluorine source. This process affords the products within a few minutes. Further reactions of such aza-S(VI) fluorides have also been investigated, disclosing their synthetic utility in the preparation of diverse S(VI) compounds.

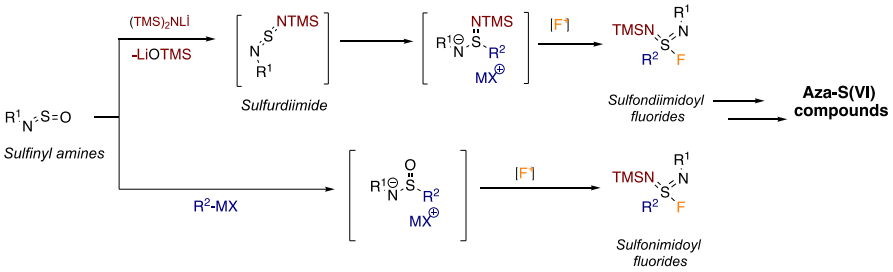

Figure 1: One-pot preparation of sulfonimidoyl fluorides and sulfondiimidoyl fluorides

Acknowledgement: *The project has received funding from the European Union's Horizon Europe research and innovation programme under the Marie Skłodowska-Curie MSCA-DN Actions GreenDigiPharma, GA N° 101073089.*

Keywords: *Aza-S(VI) Fluorides, Sulfonimidoyl Fluorides, One-pot Synthesis, Sulfonimidamides*

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Tunable Copper based slag catalyst for the production of energy vectors

Stefano Savino [a], Giuseppe Guglielmo [b], Riccardo Muolo [a], Khaja Mohaideen Kamal [c], Fiorenza Fanelli [d], Giuseppe D'Amato [b], Paolo Bollella [a], Angelo Tricase [e], Michele Casiello [d], Rosella Attrotto [b], Blaž Likozar [c], Angelo Nacci [a,d], Lucia D'Accolti [a,d]

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Steel slag, a residue from steel production, is known to contain various metal oxides and minerals that have the potential to act as green and sustainable catalysts for chemical reactions. Previous studies have already shown the possibility to enhance slag properties adding precious metals, such as palladium[1].
In this study, we synthesized a catalyst by functionalizing steel slag with copper and evaluated its performance in the photoreduction of CO_2 for the production of several energy carries such as formic acid and methanol, under simulated solar light irradiation. Moreover, the full characterization of the catalyst with XRD, XPS and SEM allowed us to obtain a tuneable catalyst with good performance both in the photoreduction of CO_2 and in the photoproduction of hydrogen.

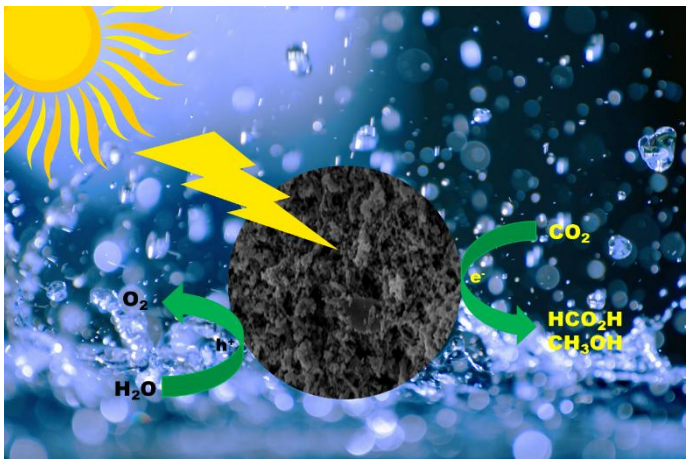

Figure 1: Schematic reaction process

Keywords: *catalysis, photoreduction, steel slag*

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Green synthesis of 2-L ferrihydrite supported on steel slags as catalyst for the reduction of nitroarenes

Francesca Derobertis [a], Maria Michela Dell'Anna [a], Nicoletta Ditaranto [b], Luca Nodari [c], Ernesto Mesto [d], Emanuela Schingaro [d], Cristina Leonelli [e], Cecilia Mortalò [f], Antonino Rizzuti [a], Carlo Porfido [g], Piero Mastrorilli [a]

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Nitroarenes are a class of environmental pollutants generated by various industrial processes such as dye and pharmaceutical production. This harmful waste[1] can be possibly valorised by reducing the nitro group to amine to obtain substituted anilines, which are highly valuable chemical intermediates. This study deals with the reduction reaction of nitroarenes employing hydrazine monohydrate as reducing agent and iron-supported steel slags as a novel heterogeneous catalyst. Steel slags (SS) are a waste product of steelmaking industry, characterised by the presences of silicates, carbonates and hydroxides[2]. SS present high alkalinity and can act as reactive support for iron, triggering the formation of catalytically active iron oxides/hydroxides, starting from inexpensive iron salts. A systematic study will be described regarding the catalytic activity of SS modified with the following salts (or mixtures): $FeSO_4 \cdot 7H_2O$, $FeCl_3 \cdot 6H_2O$, $FeCl_2 \cdot 4H_2O$. All iron-supported steel slags revealed active in the hydrogenation of nitrobenzene with the best results achieved by the catalyst prepared from $FeCl_3 \cdot 6H_2O$ (referred as **Fe3**), for which the scope of the reaction was explored. The iron species active in catalysis is the 2L-ferrihydrite.

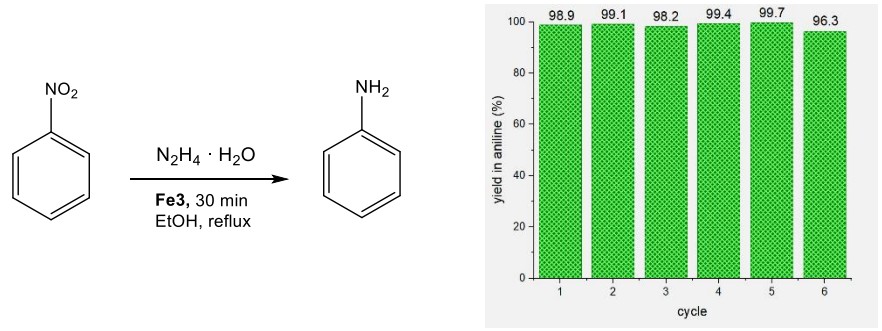

Figure 1: Recyclability of Fe3 catalyst over six subsequent nitrobenzene reduction reactions.

Acknowledgements: 10 This work has been supported under the National Recovery and Resilience Plan (NRRP), Mission 4 Component 2 Investment 1.4 – Call for tender No. 3138 of December 16, 2021 of the Italian Ministry of University and Research, funded by the European Union – NextGenerationEU [Award Number: CNMS named MOST, Concession Decree No. 1033 of June 17, 2022, adopted by the Italian Ministery of University and Research, CUP: D93C22000410001, Spoke 14 "Hydrogen and New Fuels"].

Keywords: *Steel Slags, Hydrogenation of Nitroarenes, Ferrihydrite, Mössbauer spectroscopy*

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Nanoengineered chitosan-based sponges for water remediation

Domenico Cignolo[a], Jennifer Gubitosa[a], Sara Lotito[a,b], Pinalysa Cosma[a], Paola Fini[c], Antonella Milella[a], Fabio Palumbo[b], Marinella Striccoli[c], Francesco Fracassi[a], Alberto Perrotta[b], Vito Rizzi[a]

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The presence of textile dyes and Contaminants of Emerging Concerns (CECs) in the water is a global issue because of their impact on human health and the environment. It requires great attention due to the water supply problem enhanced by global demographic increment and climate changes[1,2]. In this context, this work proposes nanoengineered chitosan-based sponges by Atomic Layer Deposition (ALD) to remove these kinds of pollutants from water, through the adsorption and photodegradation processes. In particular, a ZnO millimetric layer was deposited on the sponges' surface by ALD for making them more stable in water and able to be used as adsorbent substrates in water remediation. Moreover, the ZnO has a photocatalyst role in the pollutants' photodegradation, which is important for regenerating adsorbent material. The chitosan sponges' performances were tested on the adsorption of an azo-textile dye, the Direct Blue 78, showing a maximum adsorption capacity q_{max} of 2000 mg/g. On the other hand, Naproxen was chosen as a CEC to demonstrate the photoactivity of the deposited ZnO layer.

Keywords: *Chitosan sponges, Atomic Layer Deposition, Contaminants of Emerging Concerns, textile dyes.*

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Comparison between thermal and plasma-enhanced Atomic Layer Deposition of ZnO on fullerene powder for photocatalytic dye removal

Regina Del Sole[a,b], Fabio Palumbo[b], Francesco Fracassi[a,b], Paola Parlanti[c], Mauro Gemmi[c], Antonella Milella[a,b], Anna Maria Coclite[d,e]

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ZnO, an n-type semiconductor, possesses exemplary photosensitivity due to unique properties, first and foremost its wide band gap (3.37 eV) that leads to a strong absorption in the UV region. However, a major drawback is its fast electron-hole recombination rate that holds back the photocatalytic performances. In order to overcome this limitation, ZnO/C_{60} nanocomposites are proposed as a common solution in the literature. Indeed, fullerene can act as a co-catalyst in such nanocomposites due to its work function (4.70 eV), that allows the migration of photoexcited electrons to the energy levels of C_{60}: thus, it acts as an electron trap, increasing the lifespan of electron–hole pairs. In our work, Thermal Atomic Layer Deposition (t-ALD) and Plasma-Enhanced Atomic Layer Deposition (PE-ALD) are presented as a valid alternative to traditional wet chemistry synthetic methods of ZnO/C_{60} nanocomposites: ZnO is deposited via these two techniques on fullerene powder in a fixed bed reactor. The so obtained powders were thoroughly characterized from the chemical and morphological point of view. XPS analysis proves that ZnO grows stoichiometrically in increasing amount at increasing number of ALD cycles. The conformal deposition was successful not only on the surface of the powder grains but even on the walls of the pores of the material. In the case of thermal ALD, also deeper pores are successfully covered, while, as for PE-ALD, ZnO is found only on the walls of the most superficial ones. The photocatalytic activity of the ZnO/C_{60} nanocomposites obtained at 400 cycles by thermal and PE-ALD has been evaluated through monitoring the discoloration of a 10^{-5} M methylene blue solution upon UV irradiation over 180 min. Results indicate that the photocatalytic performance of the thermal coated C_{60} was better than the one obtained by PE-ALD (54±12% vs 33±10 %, respectively), in accordance with the higher amount of ZnO retrieved on thermal ALD treated samples.

Keywords: *photocatalysis, atomic layer deposition, zinc oxide, fullerene*

The seaweed *Chaetomorpha linum* (*Chlorophyta, Cladophorales*) as a bioremediator of microplastics

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This study represents an attempt to evaluate the presence and removal of microplastics (MPs) from the seaweed *Chaetomorpha linum* collected in the Mar Piccolo of Taranto (Ionian Sea) and then transplanted and cultivated into an integrated multitrophic aquaculture (IMTA) system, realized in the Mar Grande of Taranto including marine bioremediators such as macroalgae, polychaetes, sponges and mussels reared/cultivated around fish cages where *Dicentrarchus labrax* were farmed[1]. MPs were removed from the algae by a density separation procedure by using three extractions of hypersaline solution[2-3]. MPs were classified into different shapes, sizes and colours and some of them were analysed by attenuated total reflectance Fourier transform infrared spectroscopy (ATR-FTIR) to evaluate their chemical composition[4-5]. The collected MPs were mostly fibres (98.64%), and the predominant colour was blue (65.7%), the smallest fibre that was identified had a size of 25 µm, the largest one was 1993 µm, while the average particle size was 555 µm. The size class with the highest number of MPs was between 200 µm and 400 µm. Regarding the chemical composition, some of the analysed MPs were polypropylene, polystyrene and polyester reinforced with calcium carbonate fillers. The here realized simple procedure allowed the removal of microplastics from the seaweed, thus suggesting the potential use of the studied algal species as a food source for humans[6].

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Keywords: Bioremediation; FTIR; Macroalgae; Microplastics.

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Biohybrid Photocathode with Biobased Polymers for Green Hydrogen Production

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Microbial electrochemical systems harness the power of microorganisms to drive sustainable technologies, including biosensing, wastewater treatment, energy generation, and chemical production [1]. While significant progress has been made in identifying suitable microorganisms for these purposes, the development of efficient electrode materials remains a crucial challenge. Ideal electrode materials should possess optimal surface properties, high conductivity, and biocompatibility[2].

In this study, we leverage the potential of biobased polymers to address these requirements. Our group previously reported the use of polydopamine (PDA) coated polyhydroxybutyrate (PHB)-based electrodes for current generation. PHB, a biopolymer produced by purple non-sulfur bacteria (PNSB), offers a sustainable and biocompatible platform for bioelectrochemical systems[3].

Herein, we present the development of a biohybrid photocathode incorporating a blend of PHB and carbon nanofibers (CF), with metabolically active *Rhodobacter capsulatus* cells embedded in a PDA matrix for hydrogen production. Characterization techniques, including scanning electron microscopy, cyclic voltammetry, and chronoamperometry, revealed the significant contribution of PNSB to the observed cathodic photocurrent. This biohybrid photocathode demonstrated enhanced catalytic activity under illumination, paving the way for potential applications in water remediation and consequential energy conversion, such as hydrogen production.

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Keywords: *Green Hydrogen, Anoxygenic Photosynthetic Bacteria, Bioelectrochemical Systems, Wastewater Treatment*

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Enabling high proton conductivity in a fluorine-free protic ionic liquid through rational design of its constituents

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In the field of energy-related applications, protic ionic liquids (PILs) have attracted growing interest for their electrochemical properties and their viable preparation procedures[1]. In particular, high proton conductivity is crucial for applications such as proton exchange membranes in fuel cells. With the aim of achieving fast proton transfer through an intrinsic mechanism, we designed a novel PIL, namely *N*,*N*-diethyl-3-sulfopropan-1-ammonium hydrogen methanedisulfonate [DESPA][HMDS] (Figure 1), which is characterized by the presence of sulfonic acid moieties, of almost equivalent proton affinity, both in the anion and cation structure[2]. The electrochemical properties of [DESPA]HMDS] revealed a superionic behaviour at high temperature, as indicated by a positive deviation in the Walden plot, and by a inverse Haven ratio up to 1.55. Diffusional NMR studies revealed an unprecedented two- to three-fold increase in the mobility of the exchangeable proton, compared to that of the molecular species, again at high temperature (> 373 K). These results point towards the presence of a non-vehicular proton transport mechanism. Notably, while the best performing PILs present in the literature are often based on fluorinated or perfluorinated compounds,[3,4] [DESPA][HMDS] was designed to be fluorine-free, since perfluoroalkyl substances (PFASs) constitute a recognized concern for health and the environment, and might be subject to a ban in the European Union over the coming years[5].

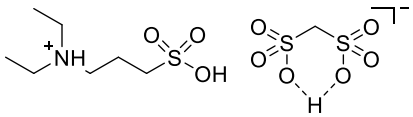

Figure 1: Molecular structure of [DESPA][HMDS].

Keywords: *protic ionic liquid, superionicity, diffusional NMR, fluorine-free*

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Thin layer bismuth vanadate photoanodes for photoelectrochemical water oxidation

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Alternative energy sources represent a sound way to tackle the climate change and pollution problems posed by the massive use of fossil fuels made by our industrialized society. Among others, solar energy is of prominent importance, because it is renewable and widely available across the world. However, it is naturally subject to intermittency and seasonal variation; thus, being able to properly store solar energy until needed is highly desirable. Within this perspective, light-driven water splitting plays a fundamental role, because it allows to convert incoming photons to hydrogen fuel.

The reactions involved in this process can take place at semiconducting materials, which ideally should exhibit the following properties: (i) absorption of a large portion of solar spectrum; (ii) favourable band edge position relative to redox species nernstian potential; (iii) low overpotential for the reaction(s) of interest; (iv) chemical stability under operating conditions [1]. Unfortunately, only a very limited number of semiconductors simultaneously fulfil all these requirements while yielding significant efficiency. Thus, many efforts are made towards the development of integrated devices and/or tandem photoelectrochemical cells, in which also semiconductor materials lacking the first two properties can be used.

In the present contribution, we report on the use of bismuth vanadate ($BiVO_4$) as a photoelectrocatalyst for light-driven oxygen evolution reaction (OER), as well as on the optimization of its performances towards this reaction.

Firstly, we will describe the synthetic route we adopted and the morphological, spectroscopic and (photo)electrochemical characterization of the as prepared $BiVO_4$ photoanodes.

Secondly, we will report on the modification of this material, known to suffer from poor electron transport within the bulk. To overcome this issue, we implemented a strategy based on molybdenum-doping, which has been proven to improve charge separation and transport within the semiconductor [2]. In the specific, we considered three Mo-doping strategies, consisting of either in-situ doping, post-synthesis doping, or a combination of both. The spectroscopic and photoelectrochemical characterization of the resulting electrodes will be discussed, in view of identifying the optimal one.

Keywords: *bismuth vanadate, water oxidation, solar fuels, renewable energy*

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Aerosol assisted atmospheric pressure plasma deposition of quercetin containing coatings for food packaging application

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Food packaging plays a key role in safeguarding foodstuffs from external factors and maintaining the highest possible level of safety and quality. In recent years, changes in production processes, retail practices and the growing demand for healthier, higher quality and longer-lasting food products has favoured the development of innovative packaging solutions, such as active packaging. Active packaging incorporates components, including antioxidants, antimicrobial agents and scavengers, and it is designed to gradually release them or to absorb other substances inside or outside the package[1]. Quercetin, a natural flavonoid with antioxidant, antimicrobial, and anti-inflammatory properties, has emerged as a promising candidate for active food packaging systems. Its incorporation into polymer matrices enhances the functional properties of packaging materials, including extended shelf life and improved safety of perishable foods[2]. Cold plasma surface modification of materials, particularly thin film deposition processes, can offer a good strategy to address these requests. Since these processes are carry out at room temperature, they can be used for the treatment of thermolabile materials such as natural and artificial polymers, or to deposit biomolecules or microorganism. These characteristics make these processes less environmental impactful and extremely attractive for industries[3]. Here we report a study on plasma deposition of quercetin-based active films for food packaging applications. Specifically, the films were deposited using aerosol-assisted atmospheric pressure plasmas. The use of this technique allows for a high deposition rate and a reduction in process costs due to the limited need for pumping systems and time. The composite films were deposited by feeding the plasma with aerosols of quercetin and isopropyl alcohol solutions using helium as a gas. (Figure 1) To better understand the nature of the deposited films, they were characterised using FTIR, SEM, UV-vis, thickness and contact angle measurements.

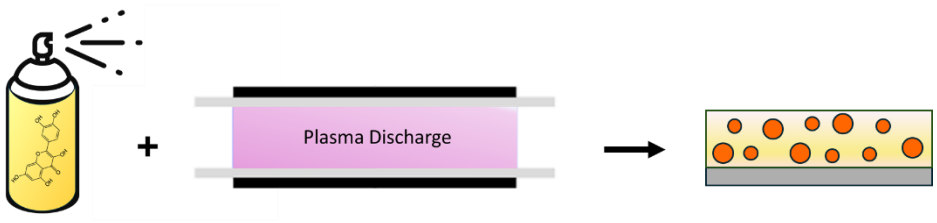

Figure 1: Diagram of the quercetin-based composite film deposition process.

Keywords: *Quercetin, active food packaging, aerosol, atmospheric pressure plasma deposition*

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A RPLC-APCI-FTMS method to characterize and quantify phytosterols in Apulian Brassicaceae vegetable products

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Phytosterols (PSs) are secondary metabolites occurring in plants in various forms, including free sterols (FSs), esters of fatty acids, steryl glycosides and acyl steryl glycosides. PSs are mainly located within the raft-domains and play an essential role in cells by preserving integrity and regulating the fluidity of the lipid bilayer[1]. PSs are bioactive substances due to their ability to lower blood cholesterol levels and to exert anti-obesity, anti-diabetic and anti-inflammatory activities[2]. In the last decade, with the increasing attention to healthy eating and lifestyle, the interest in fresh, ready to eat innovative vegetables, such as microgreens, has been on the rise. The characterization of FSs in these products using reversed-phase liquid chromatography coupled to high-resolution Fourier-transform mass spectrometry with atmospheric pressure chemical ionization (RPLC-APCI-FTMS) has thus been recently undertaken in our laboratories. The focus is on products of the Apulian *Brassicaceae* species, such as broccoli raab and kale, already known as sources of bioactive compounds[2]. In the present work, the developed RPLC-APCI-FTMS method, fine-tuned on a mixture of appropriate standards, allowed to detect FSs in extracts of microgreens, micro leaves, baby leaves and, for comparison, in the canonical mature plants of both broccoli raab and kale. Major FSs such as β-sitosterol and campesterol, as well as stigmasterol, brassicasterol and their isomers, were identified in the real samples. In particular, using HCD tandem MS, also minor isomeric species for which no standards were available were recognized. The RPLC-APCI-FTMS method was also validated to quantify FSs and thus evaluate concentration variations related to different growth stages. The obtained results show that β-sitosterol, campesterol and isofucosterol are the most abundant FSs in the examined vegetables; specific minor FSs are principally present in microgreens, thus corroborating the nutraceutical potential of these innovative vegetable products.

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Keywords:

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Determination of 2-dodecylcyclobutanone and 2-tetradecylciclobutanone in X-ray irradiated whole eggs: a green method

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The growing demand for high-protein foods has contributed to the increase of eggs consumption in recent years. However, eggs are important vehicles for foodborne illnesses mainly caused by *Salmonella*[1]. Food irradiation is a clean, safe, non-thermal technology widely used to mitigate health risk posed by pathogenic microorganisms. Currently, in Europe only the egg white can be irradiated up to 3 kGy, while the irradiation of whole eggs is not permitted[2]. Therefore, control methods to identify any illegal treatments are crucial for official inspections. The standard EN 1785:2003 method is based on the determination of radiolitic markers which are produced from triglycerides i.e. 2-dodecylcyclobutanone (2-DCB) and 2--tetradecylcyclobutanone (2-TCB). In this work, a rapid, sensitive and selective analytical method based on headspace-solid phase microextraction coupled to gas chromatography-mass spectrometry (HS-SPME/GC-MS) was applied. Unlike EN 1785, which is a time- and solvent-consuming procedure, HS-SPME/GC-MS is a fast and solvent-free method. In this study, unshelled eggs were treated by X-ray irradiator at dose levels of 1.0 and 3.0 kGy. The headspace extraction was performed using a PDMS fibre, and mass spectrometry was set in SIM mode acquisition. The analysis was done on 2.0 g of shelled homogenized egg samples placed in a 20 mL glass headspace vial containing 5 mL of deionized water. In order to evaluate the LOD of the method non-irradiated samples were spiked with 2-DCB and 2-TCB standard solutions to obtain concentrations of 1.25, 2.50, 12.5 and 25.0 μg kg^{-1}. The confirmation of 2-DCB and 2-TCB was carried out according to EN 1785:2003. Both markers were identified in irradiated and spiked samples, while no interfering peaks were found in non-irradiated ones used as control. Furthermore, a linear response was observed for both analytes in irradiated samples with increasing irradiation doses within the experimental range. A constant ratio of 2-DCB/2-TCB was also observed at different doses. Regarding LOD evaluation, the lower quantifiable level of detection was 2.50 μg kg^{-1} for both 2-DCB and 2-TCB. The preliminary results of this study, proves that HS-SPME/GC-MS method, previously applied on other foods[3], is a reliable green alternative to the official method and thus suitable in food safety control programs.

Acknowledgements: This work is supported by funding from Italian Ministry of Health who financed the Research Project IZS PB 05/23 RC

Keywords: Food irradiation, HS-SPME/GC-MS, eggs, X-ray

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Could proteins be the secret to natural rubber's high-performance properties?

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Natural rubber (NR) is the core raw material of tyre manufacturing. Its molecular structure (cis-1,4-polyisoprene) and high molecular weight (>1 MDa) give to this natural elastomer high-performing properties that cannot be mimicked by synthetic rubber[1]. A significant contribution could also be provided by the so-called non-rubber components, which make up 6% of NR. These minor compounds, including proteins and phospholipids, are linked to the linear polyisoprene chains via functional ends, forming a naturally occurring network - a complex branched structure[2].

The ability to synthesize a naturally occurring polymer is a key motivation for studying rubber biosynthesis. *Living carbocationic polymerization* occurs on rubber particle surfaces, adding isopentenyl diphosphate units to initiators and forming long NR chains encapsulated in the particle core[3]. The exact mechanism ending polymerization, which determines molecular weight, is unclear. It is suggested that the rubber transferase enzyme regulates product size and stereochemistry by recognizing prenyl chain lengths. Identifying proteins in rubber biosynthesis could help in revealing how polymer chain length is structured[4].

Mass spectrometry-based proteomics allows for the comprehensive characterization and quantification of proteins in NR. Samples from five distinct areas - southern, central, and northern Thailand, Cameroon, and Brazil - were collected. Three samples from each geographic origin or supplier were analysed for the chemometric study.

Based on proteomic findings, identifying potential correlations with the molecular weight and chain length of rubber could provide valuable insights into the mechanisms underlying linear polymer biosynthesis and the natural processes occurring during the coagulation of latex into rubber.

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Keywords: *natural rubber, Hevea brasiliensis, proteomics, mass spectrometry*

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Unlocking Nature's Palette: Enhancing Green Extraction of Anthocyanins from Apulian Pigmented Wheat Landraces

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Pigmented grains, especially those belonging to the wheat family, have recently gained attention owing to their superior nutritional and health benefits when compared to conventional varieties[1]. Being rich in several phytochemicals, such as anthocyanins, these grains are endowed with powerful antioxidant properties that can help combat oxidative stress, which is linked to a wide range of chronic diseases. As a result, pigmented grains are an excellent option for those health-conscious consumers who are progressively improving their diets with functional foods[2]. Since interest in such wholesome food items continues to grow, the potential applications of pigmented grains in both the food industry and nutraceutical markets are becoming increasingly recognized. For instance, Granomischio® offers a wide choice of grain derivatives sourced from three pigmented wheat landraces (*i.e.*, one blue bread – *Triticum aestivum* L. – and two purple durum wheat – *Triticum durum* Desf. – varieties), all cultivated in Foggia, located in the fertile region of Apulia, Italy. To date, the two most promising genotypes have been recognized as potential primary resources to produce nutraceutical supplements[3]. However, the application of acidified methanol (MeOH/HCl) sets the standard for extracting anthocyanins from pigmented grains, thus highlighting the pressing need for the development of novel eco-friendly methods to boost food security and sustainability in the food processing sector[4]. Once developing a method based on reversed-phase liquid chromatography in conjunction with ultraviolet–diode-array detector and electrospray ionization high-resolution mass spectrometry (RPLC-DAD/ESI-HRMS) to detect the main anthocyanins occurring in pigmented wheats, a strategy relying on the design of experiment (DoE) was implemented to refine a green extraction procedure. While a screening D-optimal design indicated the key factors affecting the anthocyanin extraction (*i.e.*, matrix to solvent ratio, pH, solvent composition, time, and a possible appeal to the ultrasound assistance), by a face-centered central composite design such variables were adjusted to increase the recovered amount of anthocyanins. This communication will present how the evidence provided by the DoE led to the outperformance of the MeOH/HCl with a safer alternative.

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Keywords: *Design of experiment, Pigmented grains, Anthocyanin, RPLC-DAD/ESI-HRMS*

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Enhancing Hydroponic Farming with Vermitea: A Sustainable Alternative to Chemical Nutrient Solutions

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The process of urbanization has led to the transformation of agricultural land into urban areas, resulting in a shortage of land in cities. As a result, hydroponic farming has emerged as a potential solution to ensure food security in urban areas. However, hydroponics heavily relies on mineral fertilizers derived from finite, non-renewable resources. The excessive use of chemical fertilizers, particularly those containing nitrogen, has led to elevated levels of nitrates in edible plants, posing risks to both plant growth and human health[1]. Therefore, there is a growing need to explore sustainable alternatives for nutrient solutions in hydroponic systems. This study investigates the use of vermitea, a derivative of vermicompost, as a substitute for chemical nutrient solutions in hydroponic farming. The effects of Hoagland solution, standard vermitea, and enhanced vermitea (with modified pH and electrical conductivity) on the growth and nutrient composition of *Diplotaxis muralis* were evaluated in a controlled environment (Figure 1). The results demonstrated that both Hoagland solution and enhanced vermitea resulted in higher biomass production and improved SPAD values compared to standard vermitea. Enhanced vermitea also improved the assimilation of essential nutrients, such as phosphorus, potassium, calcium, iron, manganese, copper, and zinc, while reducing nitrate levels, thereby improving the quality of plant leaves[2]. These findings suggest that enhanced vermitea can effectively replace chemical nutrient solutions in hydroponic farming, offering reduced production costs and improved product quality.

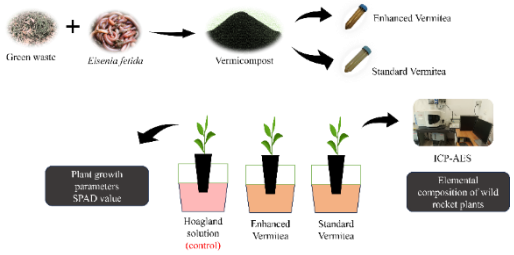

Figure 1: *Vermitea production and its effects on plant growth, SPAD value, and nutrient assimilation in hydroponically cultivated Diplotaxis muralis.*

Acknowledgements: *The authors would like to express sincere gratitude to Paolo Marini of Compost Natura s.r.l., located at Via Mallacca Zummari 32, I-73010 Arnesano, Italy, for providing the platform for preparing the vermicompost tea used in this study.*

Keywords: *vermicompost tea; rocket; organic fertilizer; sustainability*

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Phytocannabinoids profile in *Cannabis sativa* L. samples by means to LC-MRM/IDA/EPI analysis

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Cannabis sativa L. (hemp) is a dioceus plant, belonging to the Cannabacea family.1 The importance of this plant is due to the presence of specific compounds, called phytocannabinoids (cannabinoids), significant for their biological activity[1]. In this work, a new screening method was developed to detect 36 cannabinoids in 12 varieties of Cannabis sativa L. This method uses multiple reaction monitoring (MRM) combined with enhanced product ion (EPI) scanning in an information-dependent acquisition (IDA) process, performed via HPLC-MS/MS analysis. The MRM-IDA-EPI approach enabled the analysis of hemp samples and the identification of target compounds by comparing EPI spectra with literature data and an in-house library. Multivariate statistical analysis of the results provided an accurate classification of the 12 hemp varieties. The findings highlighted the important role of newly discovered cannabinoids and revealed the limitations of traditional classification methods based solely on a single common cannabinoid.

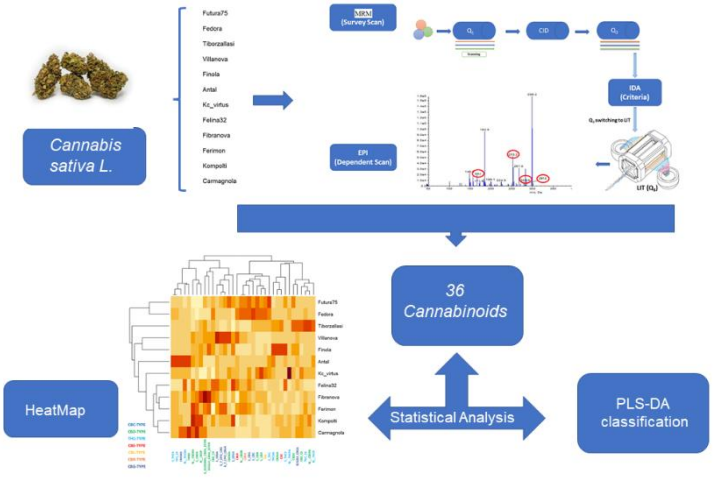

Figure 1. Scheme of phytocannabinoids and statistical approach analysis of 12 cultivars of C. sativa.

Acknowledgements: This research/publication/volume was funded the European Union – Next Generation EU. Project Code: ECS00000041; Project CUP: C43C22000380007; Project Title: Innovation, digitalization and sustainability for the diffused economy in Central Italy - VITALITY.

Keywords: *Cannabis sativa L., cannabinoids, HPLC-MS/MS, MRM-IDA-EPI, PLS-DA*

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Exploring cheese whey permeate as raw material for the chemoenzymatic synthesis of bio-based emulsifiers

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Sugar fatty acid esters (SFAEs) are a group of non-ionic surfactants which exhibited excellent interfacial tension reduction capability, biodegradability, and low toxicity. Moreover, they can be obtained from renewable raw materials, thus answering to the need of green and circular chemistry [1]. Herein, cheese whey permeate (CWP), the main waste stream of dairy industry, was used as starting material to produce bio-based surfactants. Specifically, CWP was enzymatically hydrolysed into a mixture of glucose and galactose which was then submitted to a two-step chemoenzymatic synthetic protocol (Fischer glycosylation followed by solvent-free enzymatic esterification) [2]. The first step of sugar derivatization was not straightforward since several parameter influenced both yield and isomeric ratio. Therefore, the reaction conditions were optimized thanks to a chemometric study. In the second step, an enzymatic esterification reaction was conducted leading to an isomeric mixture of *n*-butyl 6-*O*-palmitoyl-D-glycosides. The surfactancy of the obtained mixture was deeply investigated in terms of both static and dynamic interfacial tension reduction ability and water-in-sunflower oil (W/O) emulsion stabilization capacity over time [3]. Additionally, computational studies were conducted to study the role of the ring size on the final emulsifying properties of the isomeric mixture [4].

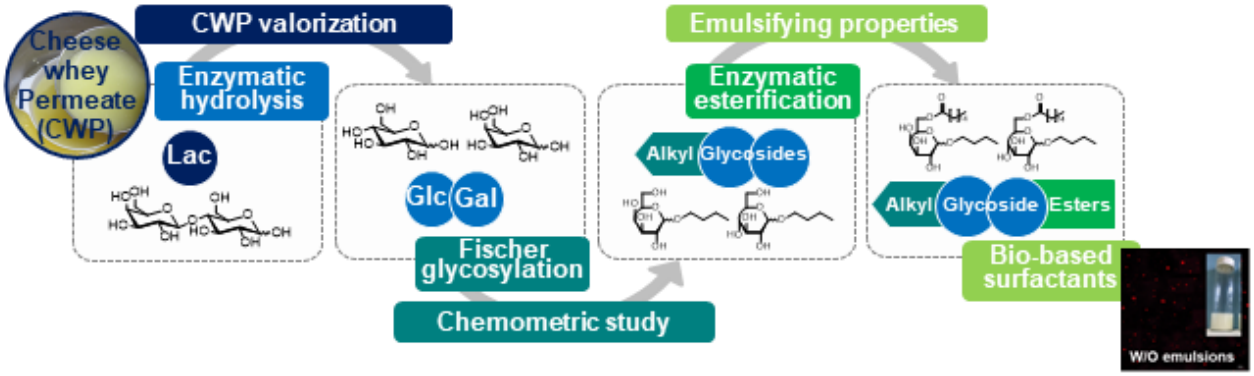

Figure 1: Chemoenzymatic synthesis of bio-based emulsifiers from cheese whey permeate.

Acknowledgements: This work has been supported by Fondazione Cariplo, grant n°2020-1094.

Keywords: *Waste valorization, bio-based surfactants, chemoenzymatic synthesis, W/O emulsions.*

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A Novel Approach to Radiochemical Determination of Ra, Th and U in Solids

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The radiological relevance of thorium, uranium and radium in solid matrices such as food, feed, soil and construction materials is an aspect of great importance to consider. These radioelements emit ionizing radiation, which can affect both human health and environment. Therefore, proper management of such materials is crucial to ensure radiological safety. Modern researches focus on various areas, including radiation characterization techniques and radiological risk assessment. The possibility of using a single method for the simultaneous determination of these three elements and their isotopes has not always been clearly established, except with methods that have relatively low sensitivity and non-radiometric methods.
This study addresses this issue using an alpha spectrometric technique consisting of three main phases: sample chemical digestion, chromatographic separation, and alpha spectrometry analysis. To enhance the method's sensitivity, food samples can be ashed in quartz crucibles (approximately 20 g) at 700 °C for 48 h, resulting in the recovery of less than one g of ash on average. The solid sample of about 1 g (soil, construction material, or ash) is then fused in zirconium crucibles with 10 g of NaOH at 600 °C for 15 min and immediately dissolved with 25 ml of ultrapure water. The resulting alkaline solution is first spiked with 40 mg of Ca and Ba, and then brought to a volume of 150 ml with ultrapure water. Subsequently, using concentrated HNO_3, the pH of the solution is lowered to 8. The solution is then centrifuged, and the precipitate is recovered with 15 ml of 1M $Al(NO_3)_3$ /3M HNO_3 solution. The second phase involves radiochemical separation of U, Th, and Ra using UTEVA chromatographic resin (Dipentyl, pentylphosphonate, or Diamyl, amylphosphonate, DAAP). The solution is passed through a 2 ml chromatographic column at a flow rate of 1 mL/min, which retains U and Th while allowing Ra and Ba to flow and elute into a clean beaker. This solution, now free of U and Th, is brought to dryness and recovered with concentrated sulfuric acid to form $[^{226}Ra]BaSO_4$ precipitate, wich in turn is dissolved in 1M HCl - 1M C_2H_5OH solution, in which $RaCl_2$ precipitates and $BaCl_2$ remains in solution. Ra precipitate is dissolved in 200 ml 0.05M HNO_3, in which a 25 mm polyethylene disk impregnated with MnO_2 is stirred for 3 h at 250 rpm on a magnetic stirrer, capturing Ra on its surface within a few µm thickness, so as not to degrade the alpha signal. Th is eluted from the UTEVA resin with 15 ml of 5M HCl / 0.05M Oxalic Acid, while U is eluted with 15 ml of 1M HCl. In each of the two eluates, the analytes are precipitated with rare earth fluorides (Cerium or Neodymium) on 25 mm polypropylene filters. The results of the tests performed on IAEA reference materials are summarized in the table below, demonstrating that the method is repeatable and suitable for the determination of the three most important natural alpha-emitting radionuclides.

Keywords: *Radium, Uranium, Thorium, chromatography*

Polyphenols as Key Markers for Machine Learning-Based Olive Cultivar Classification

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The olive tree (*Olea europaea*), widely cultivated in the Mediterranean and globally, holds a crucial role in agriculture due to the growing demand for its products, particularly extra virgin olive oil (EVOO), a cornerstone of the Mediterranean diet known for its nutritional and sensory qualities[1]. Olive fruits and their derived oils are rich sources of bioactive compounds, including polyphenols, which influence sensory properties, nutritional value, and shelf life[2]. The phenolic profile of olive fruits is highly variable and influenced by genetic, agronomic, and environmental factors, including cultivar and ripening stage[3]. This study investigates the phenolic and fatty acid profiles of olive fruits from four cultivars, such as Arbequina (ABQ), Arbosana (ABS), Frantene (FRA), and Koroneiki (KOR), collected during different ripening stages in the Abruzzo region of Italy.

The study further explores the potential of polyphenolic and fatty acid profiles as chemical markers for cultivars classification, applying machine learning algorithms such as Linear Discriminant Analysis (LDA), K-Nearest Neighbors (KNN), Naive Bayes (NB), Random Forest (RF) and Support Vector Machine (SVM). The results consistently showed superior classification accuracy with polyphenolic profiles compared to fatty acids across all algorithms. RF and SVM achieved a remarkable 98% accuracy, significantly outperforming the maximum accuracy of 65% obtained using NB with fatty acids. Including fruits at different ripening stages enhanced the dataset's robustness and the reliability of machine learning models, particularly in capturing the dynamic changes in phenolic and fatty acid profiles. The feature-important analysis of polyphenols highlighted chlorogenic acid, ferulic acid, apigenin, and pinoresinol as significant contributors to the classification model accuracy, underscoring the complex relationships among polyphenols in olive-fruit cultivar differentiation. These findings emphasize the potential of polyphenolic profiles as robust markers for cultivar identification, supported by advanced machine learning techniques capable of handling complex and non-linear data. The study highlights the growing importance of machine learning in managing complex chemical data, leading to more efficient classification methods that enhance traceability, quality control, and authenticity in the olive sector.

Keywords: *Olive fruits, Polyphenols, Fatty acids, Machine learning*

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Development of PET radiotracers for CNS diseases

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Several biomarkers have been identified as useful for the early detection of CNS diseases as neurodegenerative disorders: the efflux pump P-glycoprotein (P-gp), the sigma-1 and sigma-2 receptors (S1R and S2R, respectively) and the cannabinoid subtype 2 receptors (CB2R). **P-gp Radioligands**: The phenolic precursor FM4 (Figure 1) was synthesized to enable the two-step radiosynthesis of [^{18}F]MC225 (Figure 1A), a potent P-gp modulator currently in two different Phase II clinical trials in Netherlands[1,2]. Additionally, [^{18}F]MC225 is currently under evaluation by AIFA to initiate a new Phase II clinical trial at Gemelli Medical Center in Rome, aimed at assessing its potential for diagnosing treatment-resistant major depression. **S1R Radioligands:** Starting from L6[3], several compounds with a phenoxyalkylpiperidine scaffold (Figure 1B) have been synthesized to identify the most suitable candidate for ^{18}F-radiolabeling. Among these, one compound stands out for its high affinity for S1R and exceptional selectivity (5.36 nM at S1R vs 3009.5 nM at S2R). **S2R Radioligands**: Building on the work of Moldovan et al.[4], a pilot study investigated indole/azaindole derivatives incorporating the 3*H*-spiro[isobenzofuran-1,4'-piperidine] core (Figure 1C). While all compounds demonstrated high affinity for both S2R and S1R, none emerged as a suitable PET candidate due to a lack of selectivity. Thus, these compounds are evaluated *in vitro* for their anti-proliferative potential. **CB2R Radioligands**: A preliminary study incorporated an F-atom at various positions of a CB2R lead compound with a salicylamide scaffold (Figure 1D)[5]. Two of the synthesized compounds stood out for their high affinity and selectivity toward CB2R (5.2 nM at CB2R vs 1058 nM at CB1R, 1.1 nM at CB2R vs 2% @1μM at CB1R), making them strong candidates for subsequent ^{18}F-radiolabeling.

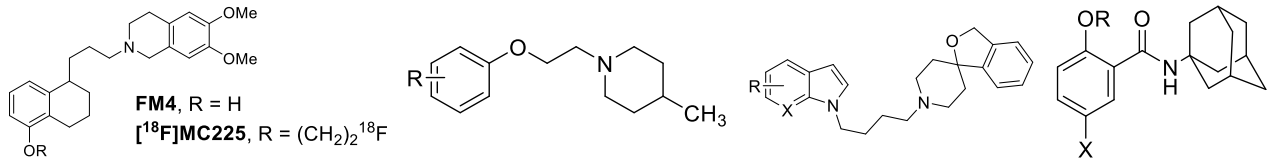

*Figure 1. General structure of PET candidate for: **A**: P-gp; **B**: S1R; **C**: S2R; **D**: CB2R.*

This work was funded by #NEXTGENERATIONEU (NGEU) and funded by Ministry of University and Research (MUR), National Recovery and Resilience Plan (NRRP), project MNESYS (PE0000006) – A Multiscale integrated approach to the study of nervous system in health and disease (DN.1553 11.10.2022), and by the National Research Council (CNR-Italy) under the program "PROGETTI di RICERCA @CNR (acronym DATIAMO).

Keywords: *PET, CNS, radiotracers.*

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Comparative Analysis of Single Molecule Transistor (SiMoT) Technology and Ultrasensitive Immunoassay Array Technologies

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Pancreatic cancer, the third leading cause of cancer-related deaths, underscores the urgent need for improved diagnostic strategies, particularly for early detection[1]. This study introduces the SiMoT (Single-Molecule with a large Transistor) platform[2,3], a promising diagnostic tool with a Technology Readiness Level of 5, designed for the early identification of pancreatic cancer precursor cysts. The performance of SiMoT is benchmarked against the commercially available chemiluminescent immunoassay SIMOA SP-X System[4,5]. A total of 39 samples, including 33 cyst fluids and 6 blood plasma specimens, were analyzed using both technologies. The SiMoT array targets a combination of oncoproteins (MUC1, CD55) and the oncogene KRAS, whereas the SIMOA SP-X system focuses on MUC1 and CD55 alone. The Principal Component Analysis (PCA) analysis (***Figure 1***) reveals that the SiMoT array effectively distinguishes between malignant or high-grade pre-invasive cysts and benign non-mucinous cysts, whereas the SIMOA assay demonstrates limited differentiation capability. Notably, SiMoT's ability to simultaneously measure protein and genetic markers at the single-molecule level in just 0.1 mL of sample fluid offers a comprehensive, reliable diagnostic approach. Additionally, the electronic output from SiMoT enables direct digital data transmission, suggesting its potential for use in field-deployable liquid biopsy applications[6].

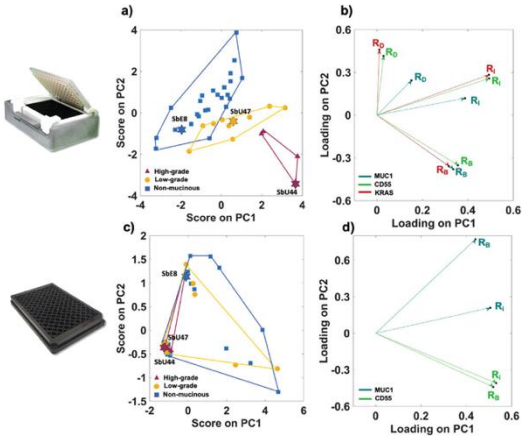

Figure 1: Multivariate data analysis of the SiMoT and SIMOA assays using Principal Component Analysis (PCA).

Keywords: *single-molecule biosensors, SiMoT-single-molecule-with-a-large-transistor, SIMOA-single-molecule-array, multivariate data processing*

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AID-CARE: Artificial Intelligence-aided Design of CAnnabinoid REceptor subtype 2 (CB2R) Multitarget ligands: a new strategy for the treatment of inflammation

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The effectiveness of drugs developed to hit inflammation may be enhanced using AI-driven systems supporting drug discovery. These systems may predict and help the development of ligands with an improved pharmacodynamic and pharmacokinetic profile simultaneously reducing the potential side effects. Cannabinoid receptor subtype 2 (CB2R), a key component of the endocannabinoidome (eCBome), plays a critical role in maintaining body homeostasis and an increased endocannabinoid tone, resulting from both direct and indirect CB2R activation. Its modulation has been shown to exert beneficial anti-inflammatory effects in inflammation-based diseases. Recently, through a "classical" computational approach, we synthesized a small series of Multi-Target Directed Ligands (MTDLs) capable of simultaneously activating CB2R and inhibiting FAAH.[1] Among the compounds belonging to this library, we identified FI5, FI8 and FI9 showing high affinity and activity at the CB2R, capable of exerting anti-inflammatory effects through reduced production of the pro-inflammatory cytokines and an increased release of the anti-inflammatory ones. Fi5, Fi8 and Fi9 displayed also some limitations such as moderate CB2R selectivity (since CB1R affinity was also present), moderate activity at the FAAH and high lipophilicity. Thus, to overcome the above-mentioned limitations of the three lead compounds, we adopted DeLA-Drug, a deep learning algorithm designed for the automated generation of drug-like analogs (applied and validated for CB2R)[2] to develop a library of novel CB2R dual drugs with an improved profile.

Figure 1: AID-CARE Project

Acknowledgement: The authors gratefully thank NextGeneration EU_PNRR_M4.C2 Investimento 1.1._PRIN-P2022TRR3Y- AID-CARE Funding.

Keywords: *Drug development, CB2R agonists, FAAH inhibition, inflammation*

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Development of an electrochemical sensor for cardiac troponin T based on molecularly imprinted nanoparticles produced by solid-phase synthesis *via* epitope imprinting approach

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Molecularly imprinted polymers (MIPs) are artificial receptors deriving from the polymerization of functional monomers around the target template, whose removal leaves complementary cavities in shape, size and functional groups in the polymeric matrix[1]. The scaling down of the imprinting process to nanosize results in the formation of imprinted cavities at the surface of the receptor, thus boosting the binding kinetics. Among the available techniques, solid-phase synthesis is based on the immobilization of target templates onto a solid support, around which molecularly imprinted nanoparticles (nanoMIPs) are synthesized and potentially employed as recognition elements for sensing applications[2]. Herein, we introduce the development of an electrochemical sensor based on nanoMIPs for the impedimetric detection of cardiac troponin T (cTnT), a valid biomarker for myocardial cell damage[3]. A short protein epitope as target template was immobilized onto the surface of glass beads, around which the polymerization was carried out. After the cTnT nanoMIPs elution, high-affinity nanoMIPs were characterized in terms of size distribution and binding properties and finally anchored *via* amide bonds onto the electrode carbon surface[4]. The as-prepared sensor was employed for the impedimetric detection of cTnT epitope and the preliminary results showed a linear response in the concentration range of 1.5 – 10 nM with a LOD of 0.09 nM, proving the sensor applicability in the Point-Of-Care testing for heart failure.

Acknowledgements: This work was partly funded by EU- Next Generation EU, Missione 4 Componente 1 CUP F53D23008850001, within the Project PRIN 2022 PNRR "HYbrid DEvices and mAchine Learning for food and environmental safety – HYDEAL4safety" (P2022T3HFA).

Keywords: molecularly imprinted nanoparticles; solid-phase synthesis; cardiac troponin t; electrochemical sensor.

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Development of Proteolysis Targeting Chimeras (PROTACs) and small molecule inhibitors for targeting neuroinflammation

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Neuroinflammation plays a crucial and complex role in brain homeostasis and is rapidly emerging as a promising target for Alzheimer's disease (AD) due to its involvement in neuronal dysfunction and death. The immune system, particularly neutrophils, contributes to neuroinflammation, since these cells can potentially either alleviating or promoting neurotoxicity through the release of pro-inflammatory mediators.[1] In the context, we have identified a hit compound showing promising inhibitory activity of a neutrophil-specific enzyme (patent pending) involved in AD neuroinflammation. This provided the suitable starting point for a medicinal chemistry campaign based on two strategies: 1) The development of hit analogs to improve inhibitory potency, selectivity, along with pharmacokinetic properties. To explore structure-activity relationships, a series of amide analogs with different substituents has been synthesized. 2) The development of proteolysis-targeting chimeras (PROTACs), which utilize the proteasome system to degrade a protein-of-interest (POI)[2], namely the neutrophil-specific enzyme. PROTACs have been designed exploiting the hit compound as POI ligand, the thalidomide as the E3 ligase binder joined via a suitable linker. A small library of PROTACs is being generated by exploring different linker lengths, flexibility, and 3-/4-positions on thalidomide scaffold to optimize chemical-physical properties and degradation efficiency. The therapeutic potential of both analogs and PROTACs is currently being evaluated in neuroinflammatory cell models of AD.

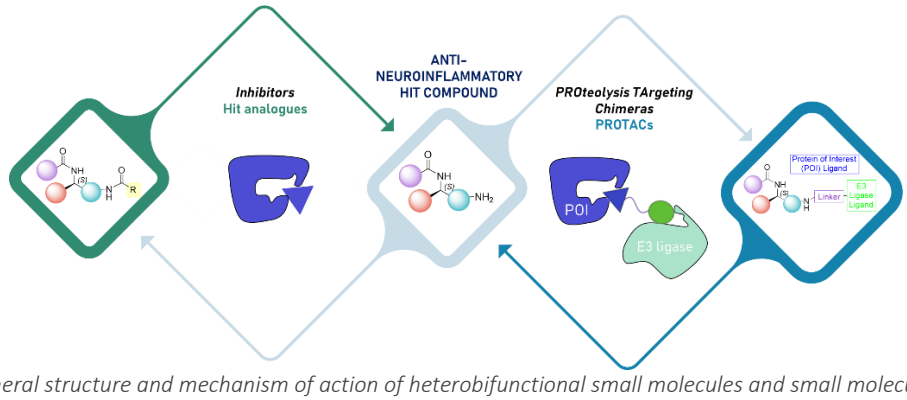

Figure 1: General structure and mechanism of action of heterobifunctional small molecules and small molecules inhibitors

Acknowledgements: this research was supported by EU funding within the NextGenerationEU-MIUR PNRR Extended Partnership 12 (Project no. PE00000006, "A multiscale integrated approach to the study of the nervous system in health and disease" MNESYS – SPOKE7)

Keywords: *Alzheimer' disease, neuroinflammation, small molecule inhibitors, PROTACs.*

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Ultra-sensitive and rapid detection of SARS-CoV-2 subgenomic RNA using a single-molecule with a large transistor-SiMoT bioelectronic platform

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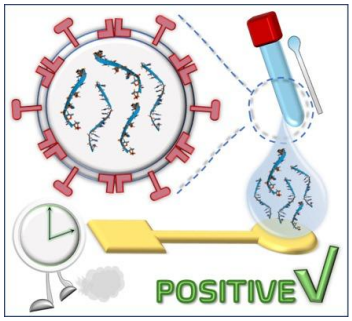
The replication of Coronaviridae viruses relies on the synthesis of structural proteins produced through the discontinuous transcription of subgenomic RNAs (sgRNAs). Detecting sgRNAs, indicative of active viral replication, offers critical insights into infection status.[1,2] However, current diagnostic methods, such as PCR-based assays, are often costly, require complex equipment, and depend on highly trained personnel. These methods can also suffer from specificity issues due to technical constraints in kit design. Although viral culture remains a gold standard for accuracy, it is impractical for routine diagnostics.[3] In this study, we introduce the Single-Molecule-with-a-large-Transistor (SiMoT) technology for detecting sgRNA encoding the nucleocapsid (N) protein in clinical samples. This technology has been shown tot detect single proteins and genetic markers (DNA or RNA) with minimal sample handling and an assay time-to-result within 1 hour, achieving a technology readiness level of 5.[4,5,6] SiMoT utilizes a stable layer of complementary DNA strands on the sensing gate electrode, allowing for the rapid, sensitive, and specific detection of sgRNAs. In a study involving 90 samples, SiMoT achieved a diagnostic sensitivity of 98.0% and a specificity of 87.8%, providing results within just 30 minutes. This user-friendly platform requires minimal sample preparation and offers a cost-effective Point-of-Care (POC) diagnostic solution. With demonstrated diagnostic accuracy and scalability, SiMoT represents a promising tool for detecting active viral replication in SARS-CoV-2 and other coronaviruses, addressing the challenges of existing molecular and culture-based diagnostic methods while enhancing access to reliable testing.



Operating scheme of the SiMoT technology for the detection of SARS-CoV-2 sgRNA, suitable for POC settings.

Keywords: *SiMoT(Single-Molecule-with-a-large-Transistor), early-detections, sgRNA, bioelectronics.*

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2- Aryloxymethylene-substituted scaffolds as privileged moieties for the design of new potential metal chelators in the multi-target therapy of Alzheimer's disease

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Alzheimer's disease (AD) is the most spread neurodegenerative disorder and, at the moment, no drugs have been approved for its treatment[1]. Different causes contribute to the onset and the progression of AD, in particular cholinergic disfunction, oxidative stress, metal dyshomeostasis and aggregation of proteins such as amyloid β (Aβ) and hyperphosphorylated tau[1]. This multifactorial origin has directed the most recent studies towards the design of new multi-target hybrids for innovative therapies[2,3].

In our last published studies, scaffolds mimicking donepezil[2] or rivastigmine[3], two anti-AD drugs, were condensed with different aryloxyacetic acids through an amide bond (Figure 1). The resulting hybrids were chemically characterized and tested against different enzymes[2,3]. Some of them, bearing nitro group in *ortho* position of aryloxy portion, showed an excellent activity as cholinesterases (ChEs) inhibitors[2,3].

In order to increase the capability of these hybrids to chelate metals (such as Cu^{2+}, Zn^{2+} and Fe^{3+}) and inhibit Aβ aggregation, while maintaining some activity against both ChEs, specific modifications have been then introduced in a new series of compounds. In this communication the preliminary results of this new challenge will be presented.

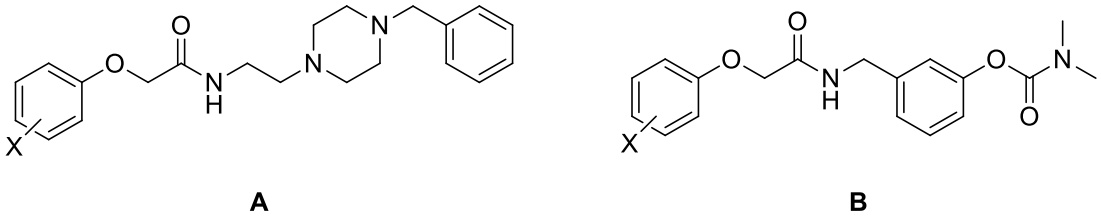

Figure 1: General structure of donepezil-like hybrids (A) and rivastigmine-like hybrids (B).

Keywords: *Alzheimer's disease, chelation, multi-target hybrids*

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Next-Generation of FPR2 Agonists: Leveraging Multicomponent Reactions to Improve Drug-Like Properties

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Formyl Peptide Receptor 2 (FPR2) is a G-protein-coupled receptor involved in innate immunity, host defense, and chemotaxis. By activating anti-inflammatory pathways through Specialized Pro-resolving Mediators (SPMs) like lipoxins, resolvins, and protectins, FPR2 plays a key role in the resolution of inflammation (RoI), a process critical for restoring tissue homeostasis.[1] Given the link between chronic inflammation and diseases such as neurodegenerative disorders, FPR2 agonists with pro-resolving properties hold promise as innovative therapeutic agents.

Multicomponent Reactions (MCRs) are efficient, sustainable synthetic methods where three or more precursors react in a single step, offering high atom economy, minimal waste, and broad structural diversity. These features make MCRs valuable for drug discovery and optimization in the pharmaceutical industry.[2]

Based on our earlier identification of non-peptidic ureidopropanamide-based FPR2 agonists with anti-inflammatory and neuroprotective properties both in vitro and in vivo models, we scouted MCRs to develop a novel series of FPR2 agonists with innovative moieties aimed at improving their drug-like properties.

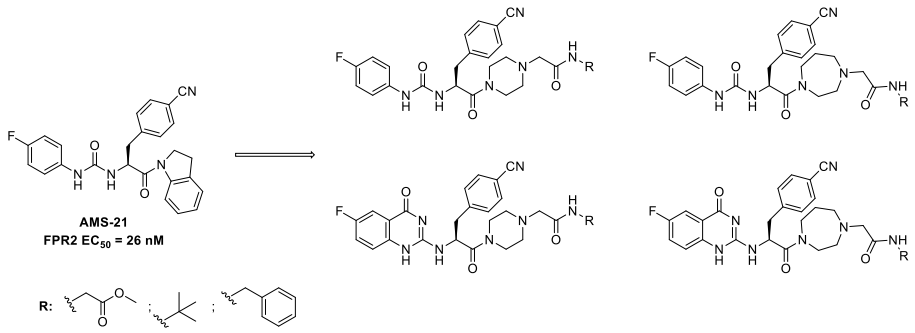

Figure 1: Development of new series of compound

Keywords: GPCR, FPR2, Ureidopropanamide, Multicomponent reactions.

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SIGMAP: an explainable artificial intelligence tool for SIGMA-1 receptor affinity Prediction

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Developing modulators for the sigma-1 receptor (S1R) offers a promising therapeutic approach for addressing neurodegeneration[1], cancer progression[2], and viral infections[3]. In this regard, in-silico tools that can accurately predict S1R binding affinity are highly desirable. In this study, we present a panel of 25 classifiers trained on a curated dataset of high-quality bioactivity data for small molecules, experimentally evaluated as potential S1R binders. All data were sourced from ChEMBL v33, and the models were developed using five distinct molecular fingerprints and multiple machine learning algorithms. Notably, most of the classifiers exhibited strong predictive performance. The best-performing model, which achieved an AUC of 0.90, was developed using the Support Vector Machine algorithm with Morgan fingerprints as descriptors. To enhance the model transparence and trustworthiness, we employed two Explainable Artificial Intelligence (XAI) techniques: the Shapley Additive Explanations (SHAP) and the Contrastive Explanation.
The top-performing model combined with the two XAI analysis is accessible via a user-friendly web platform, SIGMAP[4] (https://www.ba.ic.cnr.it/softwareic/sigmap/), specifically designed for this purpose. With its intuitive interface, strong predictive capabilities, and integrated XAI features, SIGMAP provides a powerful tool for the rational design of more effective S1R modulators.

Keywords: *Sigma 1 receptor; Ligand-based classifiers; Machine Learning; Explainable Artificial Intelligence*

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Intelligent design of novel multi-target antibiotics against superbugs

Anna Rita Tondo [a], Beatrice Marinacci [b], Ilaria D'Agostino [c], Andrea Angeli [d], Simone Carradori [b], Francesco Melfi [b], Rossella Grande [b], Micol Corsiani [d], Marta Ferraroni [e], Mariangela Agamennone[b], Susi Zara [b], Valentina Puca [b], Benedetta Pellegrini [b], Chiara Vagaggini [f], Elena Dreassi [f], Marianna A. Patrauchan [g], Clemente Capasso [h], Orazio Nicolotti [a], Fabrizio Carta [d] and Claudiu T. Supuran [d]

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Pseudomonas aeruginosa is an opportunistic pathogen responsible for severe acute and chronic infections and it has become an extensive-drug resistant (XDR) bug.[1] Herein, we present the design of multi-target compounds to tackle antibiotic resistance. In this respect, we designed 41 new ciprofloxacin-based hybrid compounds, in which the ciprofloxacin scaffold was decorated with a molecular arm enaging *P. aeruginosa* carbonic anhydrases (PsCAs).[2] These new hybrid compounds have been tested against PsCAs and human carbonic anhydrases (CA) I and II, after predicting their binding based on structure-based studies. *In vitro* testing has revealed the crucial role of spacers between ciprofloxacin and the CA inhibitor portion in influencing antibacterial activity and selectivity against various bacterial and human CA isoforms.

In silico site mapping studies prior to docking disclose within PsCA3 a possible selectivity region about 15 Å away from the catalytic site. Molecular docking unveils that this valley could represent a favorite entrance for almost all compounds into the narrow active site of PsCAs, facilitated by a particular L-shaped conformation resulted from the addition of the chemical spacer.

Promising preliminary experimented absorption, distribution, metabolism, and excretion (ADME) properties and no detected cytotoxicity endorse these ciprofloxacin derivatives as suitable candidates for the development of new multitarget antibacterial agents.

Acknowledgements: Authors want to gratefully acknowledge: COST Action EURESTOP, CA21145, supported by COST (European Cooperation in Science and Technology); the NRRP - funded by the European Union - NextGenerationEU - Mission 4 "Education and Research", Component 2 "From Research to Business", Investment 3.3; the company BioGaia AB Sweden

Keywords: *antibiotic resistance, carbonic anhydrases, molecular docking, ciprofloxacin*

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Innovative Approach to FTIR Spectroscopy: Use of Artificial Intelligence for Quantitative Analysis of the Paleolithic Site at *Riparo Mochi*

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Fourier-Transform Infrared (FTIR) spectroscopy is one of the most widely used qualitative analytical techniques. One of its primary applications is the identification and determination of the molecular composition of various organic and inorganic compounds. As FTIR has an acceptable level of accuracy and sensitivity, it should be considered among the indispensable tools for qualitative analysis[1].

In this study, FTIR spectroscopy was employed to analyse samples from one of Italy's most significant prehistoric sites, the *Riparo Mochi* in Ventimiglia (Imperia). The main aim is to study methods of construction and management of the combustion structures of the site. Through qualitative analysis, the main mineralogical phases present in the soils collected at this prehistoric site were identified. Furthermore, an innovative approach was employed to make FTIR not only a qualitative but also a quantitative technique.

A dataset of FTIR spectra was initially created by measuring KBr pellets containing known concentrations of the three primary substances identified in the samples: calcite, silicates, and quartz. To expand this dataset, machine learning techniques were applied, enabling the creation of reference spectra at various known concentrations, beyond those obtained in the laboratory[2]. As a result, by applying an artificial intelligence (AI) approach, we were able to predict the concentration of two of the three substances investigated; difficulties in producing reproducible quartz pellets hindered accurate prediction of its concentration.

As shown in Figure 1, sample 9 reveals the presence of hydroxyapatite with a low crystallinity index, which could indicate the presence of bones at the site, given that bones are primarily composed of this material. Additionally, the crystallinity index provides a means to determine the combustion temperature of the samples, offering valuable insights into whether the samples consist of burned bone[3].

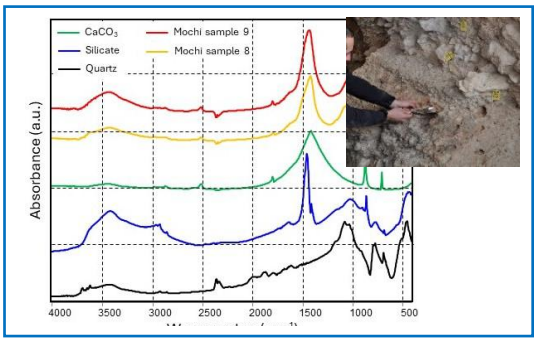

Figure 1: Example of sediment sampling at Riparo Mochi (top right) and FTIR spectra of sample 8 (yellow line), sample 9 (red line) and reference standards of calcite (green line), sodium silicate (blue line) and quartz (black line) (left).

Acknowledgements: This research is part of the project Pyro-Transitions: prehistoric cultural changes in the use of fire from foraging to the earliest farming societies, funded by MUR - PRIN 2022 (project code 2022PWY2YS, CUP Master no. E53D23000300006, CUP G53D23000310006).

Keywords: FTIR, artificial intelligence, archaeometry, neural networks

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Self-calibrated Laser Induced Breakdown Spectroscopy for in situ monitoring of Volcanic Ash.

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Volcano monitoring and hazard assessment benefit greatly from the real-time study of fine ash in volcanic plumes, which are composed of magma fragments released from the crater during explosive eruptions. Numerous analytical methods can be applied to obtain the chemical characterization of the juvenile pyroclastic material generated in volcanic plumes. Among them, the most appropriate and easily applied to advanced applications in extreme environments is Laser-Induced Breakdown Spectroscopy (LIBS)[1]. In this first part of our work, we present the elemental composition of suspended volcanic ash obtained by using LIBS experiments based on a self-calibrated technique. Different sizes of volcanic ash samples from different locations were suspended in the air by laser-induced shockwaves in a dedicated chamber to replicate the conditions of dispersed volcanic ash in the atmosphere. At the same time, a parametric study was conducted to determine the best experimental conditions for recording useful plasma emission spectra for each ash size. The quantitative analysis was then carried out via a self-calibrated analytical methodology, including Calibration-Free (CF) LIBS, that is based on the calculation of the spectral radiance of a uniform plasma in local thermodynamic equilibrium. An added asset to our analysis technique was a CF-LIBS soft that accounts intrinsically for self-absorption, since the latter modifies the intensity of spectral lines and thus leads to an underestimation of the elemental fraction [2]. In order to deduce the apparatus response from the ash spectrum itself and eliminate the need of standard calibration lamps, an intensity calibration of the spectra based on the measurements of Fe lines intensities was also used in this work [3]. The obtained results demonstrate the potential of real-time measurements of elemental fractions in volcanic ash with a good agreement with the literature composition. Now, we are planning the construction of a compact instrument that can be installed on drones for on-flight CF-LIBS measurements.

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Analytical insights into action mechanisms of ZnO-based bioactive coatings by scanning electrochemical microscopy

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The fight against antimicrobial-resistant bacteria, the increasing burden of infectious diseases, and the prevention of pandemics are just some of the concerns driving the development and widespread use of biocidal agents and materials. A comprehensive understanding of their bioactivity mechanisms and surface properties is crucial for the development of safer and more sustainable (nano)antimicrobial solutions. For example, recently our studies highlighted the importance of detailed analytical characterization in predicting potential toxicity pathways, establishing dose-response relationships for materials like Cu nanoparticles [1]. In this context, here we focus on ZnO-based materials, which are well-known for their antimicrobial properties driven by multiple mechanisms [2]. Zinc oxide exhibits bioactivity through the generation of reactive oxygen species (ROS) via photocatalytic processes and the release of Zn^{2+} ions from its surface [3]. Using scanning electrochemical microscopy (SECM) [4], we investigated these mechanisms *in situ* to determine whether ROS formation is primarily attributable to Zn^{2+} release or to the intrinsic photocatalytic activity of ZnO. The spatially resolved (photo)reactivity of ZnO-based coatings was monitored in real-time by measuring the local oxidation current of hydrogen peroxide (H_2O_2), the most stable ROS. The study begins with a detailed analytical characterization of the sub-micrometric ZnO-based materials using techniques such as transmission electron microscopy (TEM) and spectroscopic analyses (UV-Vis, ATR-FTIR, XPS). These methods provided insights into the material's morphology, chemical composition, and surface reactivity. Subsequently, SECM data revealed a correlation between localized H_2O_2 electrochemical activity and the antimicrobial surface features. A significant enhancement of oxidation currents was observed in specific micrometric regions under UV light, indicating that the activation of ZnO is a key step in ROS production. In contrast, the same current levels were not reached in the dark, suggesting that Zn^{2+} release alone results in a less consistent ROS output.

Acknowledgements: M.I. acknowledges the financial support from the ERC SEEDS UNIBA programme, project H93C23000660001, "REAL - More for less: REthinking AntimicrobiaL materials".

Keywords: zinc oxide, bioactive coatings, reactive oxygen species, scanning electrochemical microscopy

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NIR spectroscopic profiling of a progressive air purification system for indoor Cultural Heritage spaces

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Tea tree essential oil, derived from the leaves of the *Melaleuca alternifolia*, possesses remarkable antifungal and antibacterial properties, primarily attributed to its key components terpinen-4-ol. This study deals with the protection of Cultural Heritage substrates from biocolonization through a preventive approach. As fungal spores and bacteria are present in the air, they could settle-down and biodegrade works of art. So, tea tree oil might be used as a biocide to reduce the microorganisms, thus avoiding the interaction of hazardous organisms with the artistic substrate [1].

To mitigate unwanted interactions between the oil and the surfaces, as well as to counteract the inherent volatility of essential oils, the biocide was adsorbed and chemically bonded on a silica mesoporous support, i.e. MCM-41 microparticles [2].

The efficacy of the essential oil, whether attached to silica or not, is influenced by its composition, making it essential to adopt an appropriate analytical protocol. Typically, the identification of the great variety of phenolic and terpenic components of the essential oil is performed using gas chromatographic techniques, which can be time-consuming and costly [3]. In this paper we propose a non-invasive method, i.e. NIR spectroscopy, to streamline the analytical process. In fact, most essential oil substances exhibit distinct and well-defined key bands that facilitate rapid and effective characterization [4]. Additionally, the chosen support, i.e. MCM-41 microparticles, were studied in the NIR region, where the harmonic and combination bands of the fundamental modes of the surface OH groups are located.

Our investigation focuses on the changes in NIR band frequencies observed in both the silica support and the essential oil following adsorption or chemical bonding to the silica surface. This analysis aims to assess the effectiveness of the interaction between these two components, which are the heart of the purification system.

Keywords: *MCM-41, tea tree, air quality, bacteria*

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Radical Mediated Decarboxylation of Amino Acids via Photochemical Carbonyl Sulfide (COS) Elimination

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In one of a previous study of Acyl Thiol-ene ligation of amino acids and peptides recently published by Scanlan and co-workers, COS elimination was observed as a side reaction during thioester formation for di-substituted thioacids substrate.[1] To the best of our knowledge, a work published in 2016 by Shimizu et al. was the only previous example of COS elimination under radical mediated conditions available in the literature (Figure 1.a).[2] In this study we present the first examples of amino acid decarboxylation via photochemically activated carbonyl sulfide (COS) elimination of the corresponding thioacids. This method offers a mild approach for the decarboxylation of amino acids, furnishing *N*-alkyl amino derivatives. Reaction conditions were optimized for both ultraviolet (UV) and blue LED light sources. Blue LED irradiation was selected to take forward for batch synthesis since it is a milder initial energy source and can be carried out using inexpensive light sources. The methodology was compatible with amino acids displaying both polar and hydrophobic sidechains and was tolerant towards widely used amino acid-protecting groups. The compatibility of the reaction with continuous-flow conditions enables uniform irradiation, fast reaction times and efficient conversions, demonstrating the scalability of the process.

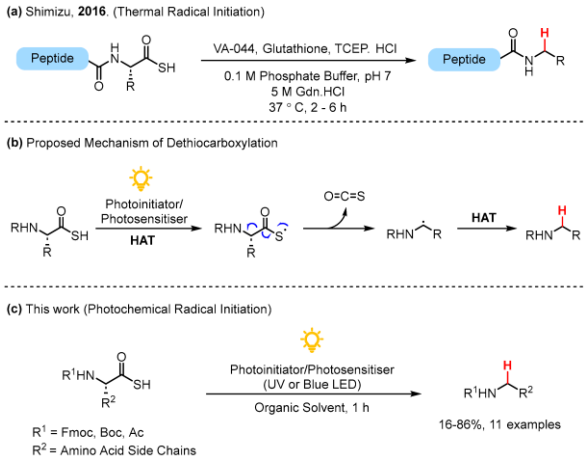

*Figure 1: (**a**) Previous work by Shimizu and co-workers [2]; (**b**) proposed mechanism of radical dethiocarboxylation; (**c**) photochemical dethiocarboxylation.*

Acknowledgements: The authors would like to thank John O'Brien and Manuel Ruether for assistance with NMR and Gary Hessman for assistance with mass spectrometry.

Keywords: *amino acid, thioacid, decarboxylation, photochemistry.*

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Green Transition In Food Authentication: G-Score Driving Method Development

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On a worldwide scale, the tomato (*Lycopersicon esculentum*) continues to increase in importance for consumption as a fresh crop and for inclusion as a major constituent in many prepared foods. Tomatoes are commonly valued not only for their sensorial properties but also for their nutritional properties due to the high content of antioxidants and bioactive compounds[1]. There are many tomato cultivars with a wide range of sensorial and morphological characteristics which determine their use. Over the last decade, several metabolomic approaches have been established to identify the differences among tomato varieties accounting for specific classes of compounds[2] but only few studies pursued authenticity purposes[3]. Following on the work presented previously[4], the aim of this study was to develop and optimize a rapid and green analytical method for Datterino purees authentication by flow injection analysis based on high resolution mass spectrometry detection (FIA-HRMS). A set of 41 commercial tomato puree samples, divided into two groups, were used for the purpose: (A) labelled as 100% Datterino, (B) low-cost alternative purees with no varietal specifications. A rapid and green metabolite extraction protocol was optimized by evaluating different parameters. The extracts were analysed by FIA-HRMS in Full scan mode switching positive/negative polarities with high resolving power on a hybrid quadrupole/orbitrap MS (Q-Exactive Plus, Thermo Fisher Scientific). The G-score of AGREE and AGREEprep software were used to drive us towards a green protocol. AGREE and AGREEprep, in fact, are tools designed for the green assessment of the analytical method and analytical sample preparation respectively. They were based on 10/12 impact categories that were recalculated into subscores on a 0-1 scale. The optimization of the protocol involved several parameters, such as extraction times, extraction solvent, amount of extracted sample, injection volume, whose effects were strictly correlated not only to the sensitivity and specificity of the final detection but also to the low environmental impact. A promising untargeted analytical approach, green and rapid (<30 min), for Datterino purees authentication by FIA-HRMS has been developed.

Acknowledgements: This research was funded by European Union-Next Generation EU, Project 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.

Keywords: Tomato authenticity, green technology, high resolution mass spectrometry, flow injection analysis.

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Future-proofing historic carbonatic and pyroclastic rocks via application of ammonium hydrogen phenylphosphonate

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The preservation of stone artifacts and monuments is a major challenge in conservation science, as geomaterials degrade through interactions with an evolving environment. Current research efforts aim to develop consolidating agents to protect these materials from common causes of decay, including water dissolution, exfoliation, fracturing, salt crystallization within the pores, stone hydric dilation due to the water absorption, and colonization by microorganisms, such as lithobacteria and fungi. These vulnerabilities are closely related to compositional and microstructural features of geomaterials, with open-water porosity being particularly significant. In Italy, the variety of stones used in historical objects and monuments is extensive, yet only a few consolidating agents are available, particularly for materials such as pyroclastic rocks [1-3]. This study aimed to explore the treatment useful for various materials with an innovative consolidant, namely ammonium hydrogen phenylphosphonate. It previously synthesized and fully characterized by microanalytical, structural, and spectroscopic means and normally specific for applications on carbonate rocks. Three lithotypes were selected: common white Carrara marble, archaeological marble sample from the early basilica of San Saturnino (Cagliari, Italy), and pyroclastic stones from the "domus de janas" of Ispiluncas-Iloi archaeological site (Sedilo, central Sardinia, Italy). The two marblesmainly consist of calcite (>95%), while the pyroclastites are porous rhyolitic volcanic rocks deriving from explosive activity and composed of a glassy pumice-cineritic matrix in which crystal-clasts, cognate fragments, and lithics are immersed. While carbonate rocks were treated solely by immersion, two application methods were tested for pyroclastic rocks, due to the low calcium content: immersion and brushing, with the latter preceded by a calcium chloride pretreatment. Treated samples were subsequently analysed by scanning electron microscopy (SEM), mercury intrusion porosimetry, powder X-ray diffraction (XRD), and FT-IR spectroscopy. Changes in hydric properties, mechanical resistance, and colorimetry were also assessed. Deposited patinas on marble effectively preserved mechanical and colour properties, confirming the compatibility of the tested ammonium hydrogen phenylphosphonate as a consolidant for carbonate stones of historical significance. For pyroclastites, both methods positively affected porosity with a decrease of its values, while brushing with calcium chloride pretreatment, notably homogenized material properties, yielding a significant increase in mechanical resistance.

Keywords: *pyroclastite consolidation, innovative materials, cultural heritage, carbonate rocks preservation*

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Aptamer-Enhanced Electrochemical Biosensor for the Detection of *Listeria monocytogenes*

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Biosensing has become a hot topic, and this is mainly to the outstanding properties of such category of sensors. Their interests ranges from the biomedical and health-care to biological and engineering fields. In recent years, a class of biosensors is continuously raising: Aptasensors. These biosensors feature aptamers, bioreceptors which demonstrated pretty good characteristics as sensing tools, such as high reproducibility, high stability, easy chemical modification, almost antibody-like affinity, extreme versatility and ease / cost-effectiveness [1]: all of these properties make aptamers viable for a great amount of applications [2]. In this work, an electrochemical biosensors was designed to detect this bacterium. A custom-made Internalin A aptamer, was used to detect Listeria monocytogenes. The aptamers were anchored to the electrodes by functionalizing the surface with a polymer, mainly polydopamine and its derivatives (i.e L-DOPA). The biosensing platform was then put to the test with different different concentrations of *Listeria monocytogenes* and a calibration curve was obtained. Rhodobacter Spheroides was also tested to assert the specificity of the aptamer. To fully study the sensors surface functionalization, electrochemical techniques such as Cyclic Voltammetry and EIS and spectroscopical techniques such as FT-IR were used.

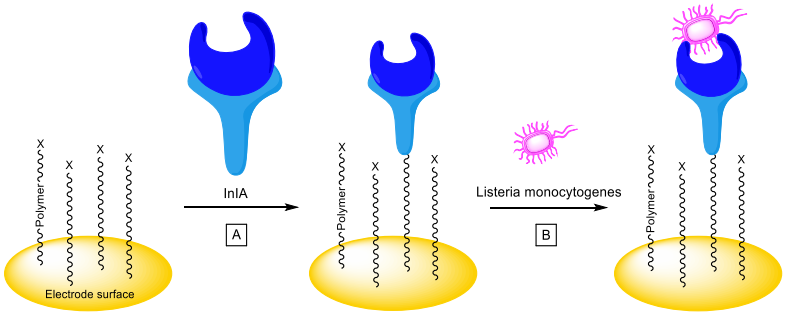

Figure 1: Scheme of mechanism involved in the biosensing process; [A] Aptamer binding to the polymer surface; [B] Listeria monocytogenes interaction with aptamer.

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***Keywords**: Electrochemistry, Biosensors, Aptamers, Polymers.*

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Thermochromic Polymeric Composite Based on 2D Hybrid Organic–Inorganic Perovskite

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Hybrid organic-inorganic perovskites (PVKs) have garnered significant attention due to their versatile chemistry, structural diversity, and advantageous physical properties [1].

This study introduces a novel thermochromic composite based on 2D PVKs. This material exhibits reversible colour switching, transitioning from a transparent state (transmittance > 80%) at room temperature to a coloured state (transmittance < 10%) at high temperatures. The reversible transition between these two states is rapid, taking only a few seconds.

Investigations involving X-ray diffraction, Fourier-transform infrared spectroscopy, differential scanning calorimetry, and optical measurements during thermal cycles revealed that the thermochromic behaviour is based on a reversible disassembly and assembly process of PVKs, facilitated by the intercalation of polymer chains. This mechanism hinges on the formation and breaking of hydrogen bonds between the polymer and perovskite [2].

By adjusting the type and concentration of organic cations in the formulation, it is possible to modulate the interaction between the polymer and perovskite, thereby controlling the switching temperature and kinetics. This research explores a novel application for PVK-based composites, paving the way for their use in thermo-responsive devices.

Acknowledgements: The author gratefully acknowledges support from the European Research Council (ERC), ERC Consolidator Grant ''HYNANOSTORE" (project number 101045746) and from the European Union –NextGenerationEU, the National Recovery and Resilience Plan (NRRP), Project code PE0000021, "Network 4 Energy Sustainable Transition –NEST" – CUP B53C22004060006.

Keywords: Hybrid organic-inorganic 2D Perovskite, Thermochromism, Thermoresponsive devices.

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Nanocellulose-based additives for paper wet strength: the interactions of chemically-modified nanofibers with commercial polyamidoamines

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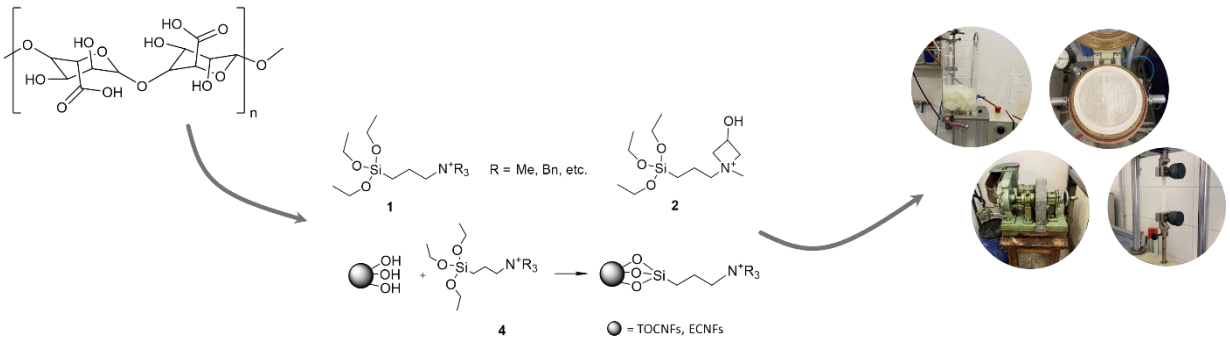
Recently, researchers worldwide have been presented with the challenge of transforming established, money-earning processes from fossil-based to green-oriented. With this perspective, the papermaking industry is trying to switch from synthetic and harmful strengthening agents to more environmentally friendly ones. In particular, wet strength is enhanced by polymer-based agents such as polyamidoamines (PAE), polyacrylamides (PAM) and glyoxylate polyacrylamides (GPAM)[1]. In this context, cellulose nanofibers (CNFs) are an optimal candidate for the reduction of these additives in the paper supply chain, given their affinity with the matrix and their well-known outstanding properties from tensile strength to high surface area[2,3].

This project focuses on the extraction and physio-chemical modification of nanocellulose to produce new bio-based paper additives. First, it was assessed whether the introduction of CNFs in the bulk phase of the paper production process increases the performance of wet strength agents, then new additives are synthesised with the aim of boosting the synergy. Since it is suggested that the main strengthening effect of commercial additives is due to the presence of positive charges on the polymeric chains[1], CNFs are produced with various methods and further chemically treated to introduce the desired moieties and giving a library of cationic materials that could mimic the behaviour of market-ready additives.



This project is funded by Mare SpA.

Keywords: *cellulose nanofibers, papermaking, strengthening additive*

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Dual-functionality starch film with conductive and antibacterial properties enabled by dicationic ionic liquid plasticizers for flexible electronics

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Over the years the use of petrol-based plastics has increased about 20 times in the last 50 years and their usage in many sectors has resulted in environmental problems. Natural polymers have been considered a replacement for common plastics, in this sense, starch is one of the most abundant polysaccharides found in plant storage organs and it is readily available. Nevertheless, starch is a brittleness material due to strong interactions among chains which confine their mobility[1]. To obtain effective starch films some plasticizers may be introduced that can improve the polymeric segmental mobility.

Recently, imidazolium-based ionic liquids (ILs) have been studied as new plasticizers due to their unique properties. In addition, ionic liquids, besides acting as plasticizers, can impart several useful properties to prepared films due to their antioxidant, antibacterial and conductive activities[2]. Lately, dicationic ionic liquids (DILs), a new category of ILs family, attracted great concern as it represents an interesting variation of the cationic partner.

In this work, the influence of the type and the length of the linkage chain on film properties will be discussed through different techniques

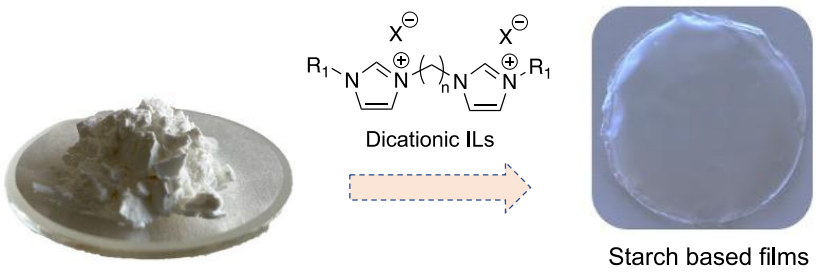

Figure 1: Plasticizing effect of DILs in producing starch-based films

Keywords: *Flexible electronics, Ionic liquids, Starch*

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Barrier performances of cellulose nanofibers-based coating agents in paper industry

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Due to environmental concerns, nanocellulose has recently become one of the bio-based sustainable alternatives to the currently used fossil-derived packaging additives, to enhance barrier properties of paper against gases, oil and water [1]. Cellulose, the most abundant biopolymer on Earth, is renewable, non-toxic, biodegradable and its hierarchical structure allows the extraction of nanoscale constituents. Among the various nanocellulosic materials, cellulose nanofibers (CNFs) are increasingly gaining attention in the field of packaging for barrier purposes. Indeed, the high hydrogen bonding ability allows the formation of a dense network, which makes it difficult for various molecules to pass through. In addition, the large surface area and the presence of a large number of hydroxyl groups, which grant the possibility to tune their hydrophilic nature, make cellulose nanofibers a promising material for the formulation of coating agents capable to enhance barrier properties of paper. CNFs can be extracted from natural sources by combining a chemical or enzymatic pre-treatment with mechanical processes. 2,2,6,6-tetramethylpiperidine-1-oxyl (TEMPO)-mediated oxidation is the most commonly applied chemical treatment which leads to the regioselective conversion of C6 primary hydroxyls to carboxylic ones. On the other hand, enzymatic hydrolysis pre-treatment of pristine cellulose, conducted with endoglucanase, results in the cleavage of glycosidic bonds, leaving the chemical structure of cellulose backbone unmodified. Both the pre-treatments have the advantage of reducing energy consumption during the mechanical process, which is the actual nanosizing step. In this work CNFs are extracted through two different methods to compare barrier properties of different coating agents, which are formulated varying several parameters. Two different paper matrices (recycled and food-contact paper) are tested, while CNFs-based coating agents are applied through spray coating technique. Oil, water and air resistance are evaluated and promising results, notably in terms of oil and air resistance, are presented.

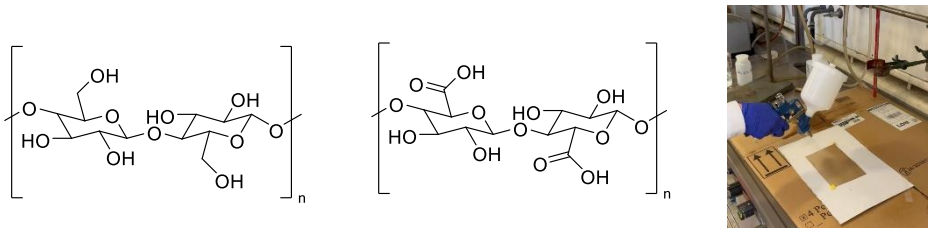

Figure 1: from left to right (i) Chemical structure of enzymatic cellulose nanofibers (ii) Chemical structure of TEMPO-oxidized cellulose nanofibers (iii) Spray coating process

Acknowledgements: This project is financed by Mare S.p.A

***Keywords**: cellulose nanofibers, barrier properties, paper industry*

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Versatile vapor-phase MIP deposition on nanostructured $PSiO_2$ optical transducer for label-free quercetin sensing

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In recent years, there has been significant progress in the development molecularly imprinted polymers (MIPs)-based sensing devices driven by their low cost, high selectivity and durability. MIPs are synthetic materials with properties specifically tailored to target analytes. One of the key factors contributing to the attractiveness of MIPs for sensing device fabrication is the wide variety of monomers available for synthesizing MIP matrices, which can be carefully selected to suit different transducing systems[1]. However, despite the huge progress in polymerization techniques, the fabrication of MIPs on complex transducing systems is still challenging. Proposed versatile techniques are dopamine polymerization and electro-polymerization, but the first is difficult to control for its inherently self-aggregation and the latter is not applicable to non-conductive transducers. The iniferter polymerization techniques are very promising providing tight control over polymer features. Nevertheless, the approach is sensitive to oxygen that can quench the radicals generated by the iniferter, requiring an inert atmosphere or additional precautions during the synthesis. Moreover, when using the light as triggering agent, the solvent must be transparent, which can restrict solvent choices. For these reasons, a simple and rapid polymerization technique for MIPs synthesis is still required. Here, we propose a room temperature vapour phase deposition of MIPs on nanoporous silicon ($PSiO_2$) scaffolds, used as challenging optical transducer, for their complex geometry. Pyrrole was used as functional monomer leveraging its ability to vaporize at ambient pressure and temperature[2] to obtain a new MIP for quercetin (QU), chosen as target. Prior to the polymerization, QU was anchored on the transducer surface by a naïve carbodiimide linker. After an optimization procedure a polymer deposition step of 30 minutes is sufficient to obtain a sensitive MIP. The resultant sensor can detect QU target within a wide concentration range from 2.5 to 200 μM, with satisfactory reproducibility (RSD=15%) and repeatability (RSD=7%). Moreover, the sensor remains functional for at least 60 days when stored under ambient conditions without requiring special care. Quercetin detection in real samples of red and white wines was validated using High-Performance Liquid Chromatography (HPLC), demonstrating the robustness of the optical sensor. The proposed approach is highly versatile, offering potential adaptability to a wide range of transducers and target molecules due to its simplicity and precise spatial control over the polymer's features.

Acknowledgements: This work was partially funded by the European Union Horizon Europe program under grant agreement No 101046946 (RESORB).

Keywords: *vapor-phase deposition, molecularly imprinted polymers (MIPs), porous silica interferometers, quercetin.*

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Timeless Questions and Modern Challenges: Exploring the Origin of Life and Electrochemical CO_2 Reduction

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Since the discovery of the first Oceanic Hydrothermal Vent field in the 1970s, these geological formations have been proposed as possible cradles for the emergence of life on our planet. In the Archean era, at the Alkaline Hydrothermal Vent environment, a mineral barrier, composed of iron oxide and hydroxide, iron sulphide, along with Ni, Zn, Co, and Mn ions precipitate creating the vent structure itself. This mineral barrier separates two different environments: the outer acidic with CO_2 and the inner alkaline with H_2, in this situation an electrochemical potential difference is generated across the vent structure; this energy can be dissipated through coupling of CO_2 reduction reaction with hydrogen oxidation, generating the very first organic molecules on our planet. [1]

On the other hand, material scientists and chemists worldwide are frenetically searching for an effective material capable of performing CO_2RR at affordable prices. Could the Fe-based minerals that performed carbon dioxide reduction 4.4 billion years ago be utilized in today's industry to address the environmental challenges of the new millennium? Here is the idea of "emergence of life inspired material" for CO_2 conversion.

Recently, a new approach to the study of Hydrothermal Vents has emerged from electrochemistry[2,3]. In our research[4] , Mackinawite (Fe-S) and Violarite (Fe-Ni-S) based electrodes have been prepared, characterized and tested by performing electrolysis in a CO_2 environment, revealing the production of formic acid, methanol, and carbon monoxide at -0.72 V vs RHE (HCOOH and MeOH had never been identified before on such materials).

The geological system is modelled as a fuel cell where a continuous supply of carbon dioxide and hydrogen is provided. The electrode material is composed of the vent's minerals, with the anode and cathode short-circuited in a configuration that recall a corrosion process. The system, capable of coupling CO_2RR and HOR (or other oxidation process), is ultimately powered by the pH difference between the two compartments (simulated inner vent fluids and oceanic waters). An electrochemical analogue of the vent has been created in an H-type cell to study the current and electrical potential trends during operation. The results are then compared using an Evans-type diagram.

Keywords: *CO_2 Reduction, electrochemistry, origin of life, hydrothermal vent*

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Electric Field Cycling Enhances Stability and Reduces Polarization Dispersion in Physisorbed Antibody Biolayers

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The analysis of the dielectric properties of proteins, particularly in biolayers, is crucial for applications in bioelectronics and sensing. Antibodies, with a non-zero electric dipole moment (μμμ), respond to external electric fields (EF)[(1)] . When deposited on a substrate, they form a biolayer characterized by a spatial distribution of dipoles, where the net dipole moment per unit volume (PPP) defines the dielectric properties of the film. These properties can be measured using techniques such as Kelvin Probe Force Microscopy (KPFM) [(2)], which detects the surface potential.

The reproducibility of PPP is essential for bioelectronic applications.

Biolayers containing antibodies covalently bound to biosensing surfaces are considered more stable, but surface physisorption offers advantages such as ease of fabrication and high stability. This study investigates the effects of electric field cycling (EF-cycling) on anti-IgM biolayers physisorbed on gold (Au). EF-cycling reduces the dispersion of PPP values across 31 samples while maintaining a constant median, thus improving reproducibility. Moreover, EF-cycling acts as an "annealing" process, leading dipoles to a more stable and statistically probable conformational state[(3)].

These findings provide new insights into the mechanisms of dielectric rearrangement in biolayers and enhance understanding of their properties. This knowledge supports the development of innovative strategies for bioelectronic devices with stable and reproducible biolayers.

Keywords: *Kelvin-Probe-Force-Microscopy (KPFM), protein-physisorption, Single-Molecule-With-a-Large-Transistor(SiMoT), zeta-potentials*

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Effect of chemical structure and electrolyte on the electrochemical energy storage properties of quinone derivatives

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In recent years, organic redox molecules have gained significant attention as promising materials for making sustainable lithium battery cathodes. Compared to metal-based active materials, organic active materials offer many advantages: they are abundant, less toxic, biodegradable, and easy to be produced and chemically modified to enhance performance [1].

Quinone derivatives are widely used as storage materials due to their reversible two-electron redox reaction and their high-operating voltage (2-2.8 V vs $Li|Li^+$) [2,3].

This study investigates the electrochemical behaviour of three quinone-based molecules [4]: p-benzoquinone (BQ), 9,10-anthraquinone (AQ), and 2-hydroxy-1,4-naphthoquinone (HNQ) (Figure 1).

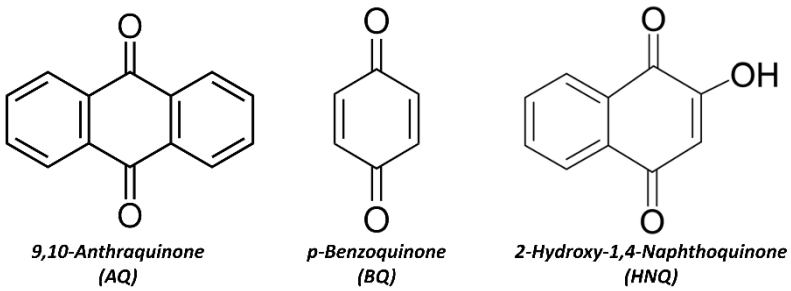

Figure 1: Simple quinone-based molecules selected.

The effect of the chemical structure, electrolyte salt ($LiClO_4$ or $TBAPF_6$), and solvent on their electrochemical storage properties are explored.

The electron-transfer kinetics and its variation are evaluated by the half-wave potentials ($E_{1/2}$) extracted from cyclic voltammetry (CV) performed at various scan rates. It is found that the donor number (DN) of the solvent affects the binding probability and strength with Li^+, thereby influencing the solvation environment. Furthermore, the size of the cations (Li^+ or TBA^+) plays a significant role in the reduction process.

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Keywords: Redox Molecules; Quinones; Organic Batteries

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Superabsorbent Hydrogels Based on Pectin and Succinic Anhydride

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Superabsorbent hydrogels (SAPs) are hydrophilic polymers properly cross-linked, which can absorb from up to 1000 times their own weight[1]. Nowadays, the most used SAPs are based on non-biodegradable and fossil-based polyacrylic acid, which possesses extraordinary swelling performances, due to the high presence of carboxylate. This work aims to produce a biodegradable carbohydrate-based polymer, opportunely modified introducing ionisable pending groups. The chosen reaction is succinylation. In the literature, there are several examples of succinylation of different polysaccharides such as cellulose[2], guar gum[3], etc. but, to the best of our knowledge, no data have been reported on pectin. Therefore, pectin succinate was synthesized from succinic anhydride and pectin in water in the presence of 4-dimethylaminopyridine (DMAP). The structure of the product was confirmed by FT-IR, ^{1}H-NMR, and ^{1}H-COSY-NMR spectroscopies, while the thermal properties were studied by TGA and DSC analyses. The main evidence of succinylation was the comparison of NMR spectra of the product and a succinate galacturonic acid sodium salt, synthesized in the same experimental conditions, in order to carry out a model reaction. To improve mechanical proprieties, the succinate pectin was cross-linked by $CaCl_2$ and $MgCl_2$ and the absorption and retention of saline solution were measured. This study demonstrated a valuable way to synthesize pectin-based hydrogels with improved gel characteristics.

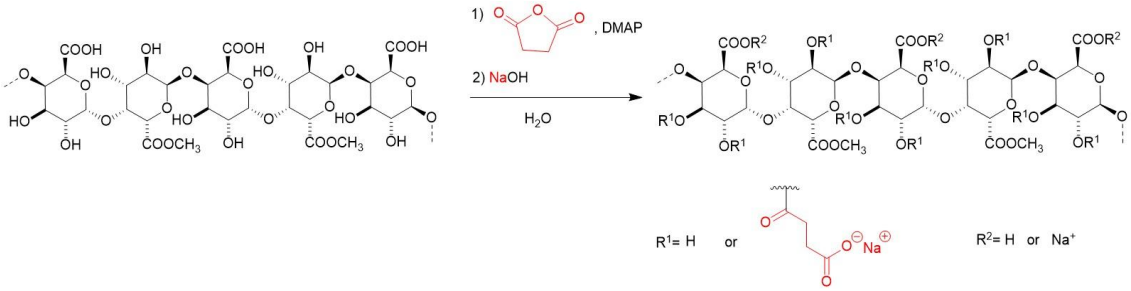

Figure 1: Scheme of succinylation reaction performed on pectin.

Keywords: *Pectin, succinylation, hydrogel, water retention*

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Carbon-Based Materials and Microfluidic Platforms for Neural Tissue Regeneration: Towards Integrated In Vitro Models for Brain Repair

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Regeneration of the central nervous system (CNS) remains one of the greatest challenges in neuroscience, with limited therapeutic options currently available. Carbon-based materials (CBMs), such as carbon nanotubes (CNTs) and graphene, have emerged as promising tools to support neuronal repair, demonstrating the ability to modulate synapse formation and cell excitability[1]. Moreover, to fully explore their potential, innovative *in vitro* models are needed to recreate the complex microenvironment of neural tissues and provide insights into mechanisms of regeneration.

In this study, two types of Carbon Nanotubes (CNTs), differing in length but with comparable diameters, were functionalized via 1,3-dipolar cycloaddition to enable deposition on substrates while preserving their conductivity properties[2].

Glass substrates were coated with functionalized CNTs and subsequently defunctionalized to restore pristine-like characteristics. These materials were characterized using electron microscopy (SEM, TEM), thermogravimetric analysis (TGA) and contact angle measurements.

The effects of these substrates on primary chick neurons cultures were investigated focusing on how CNT morphology influences neuronal network formation, assessed through electrophysiological and immunofluorescent techniques.

In parallel, we developed an Organ-on-a-Chip (OoC) platform with passive microfluidic channels modified with CBMs to enhance hydrophobicity and antifouling properties enabling the study of cellular crosstalk in the neurovascular unit (NVU).

Future work will integrate CNT-functionalized substrates into the OoC platform to investigate CBM-driven effects on neuronal regeneration and neurovascular interactions, advancing understanding of CNS repair mechanisms and their applications in traumatic brain injury and other disorders.

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Keywords: Carbon nanotubes, Graphene, Neurovascular Unit, Brain disorders

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Luminescent Zero-Dimensional Inorganic Perovskite-Photocurable Resin for Scintillator

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The preparation of perovskite-polymer composites is one of the most effective ways to improve the stability and expand the application of inorganic perovskite[1]. Resin formulations based on monomers that undergo photopolymerization induced by UV irradiation can be an intuitive method to achieve complex geometries with desired functions. In this regard, the inclusion of filler sensitive to radiation can be an immense step toward realizing customized devices for detecting high-energy radiations with advanced geometries and improved resolution. To achieve this, scintillating materials that can transform high-energy photons or electrical charges into low-energy photons can be implemented into resin formulations[2]. The superior photophysical and electronic properties of metal halide perovskite, including large absorption coefficients, high photoluminescence yields, fast decay time and structural stability make them promising candidates for next-generation scintillator. This work aims to develop inorganic perovskite polymer-based nanocomposite suitable for stereolithography fabrication for creating scintillators with high detection power and desired geometries. An all-inorganic 0D lead halide perovskite-based powder, Cs4PbBr6, is used as the scintillating material (filler) due to its large stopping power, high quantum yield, large bulk resistance, and fast response. Different precipitation methods, as the ratio of the precursor and the antisolvent used, were performed to obtain a stable powder with a strong green emission (-515 nm). 'Genesis-Development resin Base' manufactured by Thethon 3D is used as polymeric matrix of the nanocomposite. The curing process of the nanocomposite was studied by thermal analysis, in detail Differential Scanning Calorimetry (DSC), to investigate the influence of the perovskite-based powder on the cross-linking of the resin. Photo-DSC was used to study the rate and the enthalpy of crosslinking of the samples compared with the dynamic DSC study on UV lamp cured samples with the aim to calculate the ratio of curing to optimize the process for the developed formulations. By using photo-DSC, the resin material showed improved photopolymerization in presence of perovskite powder with a normalized enthalpy of crosslinking of 485 Jg-1 compared to 380 Jg-1 of the pristine resin material. Photoluminescence, Diffuse Reflectance and X-Ray Diffraction measurements gave the characteristic peak of the Cs4PbBr6, and the Fluorescence lifetime measurements showed no alteration of the lifetime which further confirms the stability of the perovskite in the composite. The excellent results assert the possibility of using the developed perovskite-polymer nanocomposite formulation as a good photocurable scintillating material

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Camphorsulfonic-Salified Chitosan Allowing MACl-Free Stabilization of Pure $FAPbI_3$ α-Phase via Gravure Printing in Ambient Air

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Metal–halide perovskites have gained extreme interest in the photovoltaic field[1] with formamidinium lead iodide ($FAPbI_3$) currently being one of the best performing materials for single-junction solar cells. Despite the outstanding record efficiencies, there are still several major issues hindering the large-scale fabrication of perovskite solar cells. The vulnerability to environmental agents[2] along with the need of controlled atmosphere and crystallization aids for the perovskite film deposition represents the major roadblocks[3]. This is particularly true for $FAPbI_3$ for which the thermodynamically stable phase at room temperature is photovoltaically inactive δ-phase. To address those challenges, herein, a camphorsulfonic-salified chitosan is specifically designed with the aid of DTF calculations to strongly interact with the perovskite and, as a result, to improve the morphology and optoelectronic quality of the $FAPbI_3$. The polymer with hydroxy and amino functional groups establishes ionic and hydrogen bonding interaction with the organic cation of the perovskite and acts as a template to assist the perovskite growth, controlling the morphology of the perovskite films and consequently reducing defect states, which are crucial in terms of degradation of the material. Moreover, the long hydrophobic chains of the polymer provide an enhanced environmental stability against moisture, light and heat, as well as higher mechanical strength. Furthermore, the addition of the polymer allows a precise control on the rheology of the solution, which is a critical factor for large-scale deposition techniques. Thanks to the numerous interactions and the modulation of the solution viscosity, $FAPbI_3$ devices are fabricated by gravure printing deposition with low-toxicity DMSO as only solvent without either antisolvent bath or inclusion of methylammonium chloride (MACl) as additive. The gravure-printed devices with the chitosan feature an enhanced efficiency and stability in air, retaining 80% of the original efficiency after 1200h in ambient air without any encapsulation.

Keywords: *Ambient air deposition, Perovskite solar cells, Polymeric additives.*

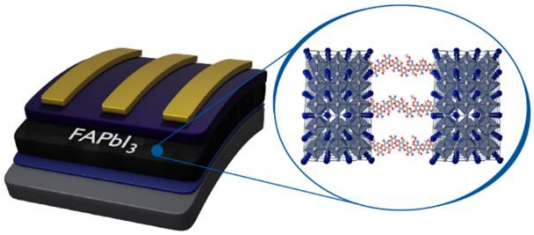

Figure 1: $FAPbI_3$ perovskite solar cell with salified chitosan

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Plasma-treated thermoresponsive hydrogels as RONS delivery systems for colorectal cancer therapy

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Cancer treatment with Cold Atmospheric Plasma (CAP) has emerged as a promising, less toxic alternative to conventional anticancer chemotherapy, either through direct application or via plasma-treated liquids or hydrogels. CAP's therapeutic effects are primarily attributed to its generation of Reactive Oxygen and Nitrogen Species (RONS) at room temperature, in a controlled and tunable manner[1,2]. When properly administered, these species induce oxidative stress, promote cancer cell death, and stimulate antitumor immune response[1,2]. This study focuses on the plasma processing and the chemical characterization of Plasma-Treated Pluronic F127®-based Hydrogels (PTHs) as novel RONS delivery systems for the local treatment of colorectal cancer, one of the most prevalent and lethal cancers worldwide[3]. Pluronic F127® is a synthetic, amphiphilic triblock copolymer known for its excellent biocompatibility and low immunogenicity, making it ideal for clinical applications[4]. Additionally, it forms thermoresponsive physical gels[4], which make PTHs suitable for local injection in their liquid form, offering a controlled release of RONS at the tumour site after gelling at body temperature. In this study, Pluronic F127® was dissolved in Electrolyte Rehydrating III Solution (SIII) supplemented with the phenolic amino acid L-Tyrosine (SIII-Tyr), as it has demonstrated a pro-oxidant effect[2]. Plasma exposure of the polymeric solutions enriched them with RONS, whose concentration and typology changes as a result of the experimental parameters used. CAP treatment was carried out using a dielectric barrier discharge (DBD) fed with pure O_2 or synthetic air. RONS release from the hydrogels was monitored over time, demonstrating a controlled and effective release profile. Preliminary in vitro analyses further support the potential of these plasma-treated hydrogels as a promising application in cancer therapy.

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Keywords: *Cold Atmospheric Plasma, Thermoresponsive hydrogels, Pluronic F127®, Oxidative stress.*

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Novel Hybrid Nanocomposites based on Au Nanoparticles decorating Viticulture Biomass-derived Graphene Oxide and Soot Carbon Waste Nanoparticles

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The urgent demand for decarbonizing the environment requires advancements in research and innovation within the frameworks of sustainable development and circular economy. This involves devising novel, sustainable strategies in material science[1] for recycling and upcycling by-products, such as biomass from agriculture sector or soot carbon nanoparticles (NPs) from incomplete combustion of industrial wastes, into high-value-added materials. Valorisation of biomass is an eco-friendly pathway that gives renewed purpose of carbon-rich by-products[2], allowing production of graphene oxide (GO). On the other hand, soot carbon waste NPs contain a graphitic carbon atom content depending on their combustion conditions. These secondary raw materials can be conveniently used as versatile platforms for further functionalization with inorganic nanostructures having different chemical composition, opening the venue to the development of multifunctional nanocomposites, promising for diverse advanced applications. Recent studies, in fact, have demonstrated the potential of biomass-derived GO and soot carbon waste NPs as scaffolds for decoration with metal NPs for catalytic, sensing, and environmental applications, with green synthesis approaches, offering sustainable strategies for waste reduction[3,4]. This work reports on sustainable colloidal chemical routes for synthesizing hybrid nanocomposites formed of Au NPs and GO, derived from viticulture biomass by pyrolysis, and SOOT carbon waste NPs, achieved from combustion of hydrocarbon fuels. The resulting hybrid nanocomposites are dispersible in aqueous solutions and their spectroscopy, structure and morphology properties were characterized. The combination of renewable sources with Au NPs is a promising strategy for manufacturing new added value state-of-the-art hybrid nanocomposites by eco-friendly routes, avoiding the use of commercial and more expensive graphene derivatives based scaffolds[5], addressing environmental sustainability and technological innovation.

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Keywords: Graphene Oxide, Soot nanoparticles, Gold Nanoparticles, Hybrid Nanocomposites

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Large Pores Mesoporous Silica-Based Nanostructures and Nanostructured Lipid Carriers as Promising Nanotools for Gene Transfection in Cancer Immunotherapy

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Tumor immunotherapy has seen a dramatic resurgence of interest due to the development of T cells genetically engineered (Chimeric Antigen Receptor T (CAR T) cells) to express the synthetic CAR to recognize antigens directly on the tumor cells surface, allowing them to attack cancer cells with greater effectiveness. CD19 is considered a highly specific target because it is found on most B cells malignancies, so by engineering T cells to express CARs that recognize CD19, these modified T cells can selectively eliminate CD19-expressing cancer cells, leading to remission in many patients with refractory or relapsed cancers. To advance gene-modified cell therapies, lenti- or retroviral vectors are employed although these approaches are costly and characterized by residual risks such as germline transmission, immunogenicity, and insertional mutagenesis. Therefore, there is a quest for efficient strategies for non-viral transduction of synthetic receptors into primary T cells able also to protect the genetic material from the premature degradation by enzymes [1]. Synthetic nanovectors, loaded with a specific plasmid (pSLCAR-CD19-28z), have been explored to bypass chromosomal integration, reduce risks and avoid enzymes degradation. Here, nanostructured lipid carriers (NLCs) and large pores mesoporous silica nanoparticles (MSNs) were synthesized for their advantageous properties, including biocompatibility and efficient loading capability. NLCs were produced through the hot homogenization technique and loaded with the plasmid using a hydrophobic ion pairing approach. MSNs were synthesized *via* dynamic soft-templating and single-step sol-gel processes, respectively and were surface-functionalized with a cationic polymer polyethyleneimine (PEI) for plasmid loading. The physical-chemical characterization and *in vitro* studies of both nanostructures revealed an average hydrodynamic diameter lower than 200 nm, demonstrating excellent colloidal stability in physiological media, efficient plasmid release without degradation and good biocompatibility. These findings highlight the successful development of these nanoplatforms positioning them as promising candidates for potential applications in oncology.

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Keywords: *nanostructured lipid carriers, large pores mesoporous silica nanoparticles, gene delivery, cancer immunotherapy*

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Versatile Conductive Ink Formulations for Flexible, Wearable, and Edible Enzyme-Based Biosensors

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Conductive inks play a key role in the development of disposable electrochemical sensors, allowing the fabrication of screen- and stencil-printed electrodes with performance comparable to solid electrodes [1,2]. In this study, biocompatible inks were developed and stencil-printed onto flexible supports. These supports are designed for easy integration into smart devices, enabling continuous and minimally invasive monitoring of lactate and glucose levels.

The formulation of the conductive ink was optimized through electrochemical and rheological measurements, using a multivariate analysis model to refine its properties. The active carbon electrodes were then modified with osmium redox polymers (ORPs), which facilitate electron transfer between the electrode and enzymes such as glucose oxidase (GOx) and lactate oxidase (LOx), as these enzymes cannot directly transfer electrons [3,4]. The biosensors were tested in both model solutions and sweat to assess their performance and analytical reliability.

This research has the potential to make edible biosensors. These devices can detect a wide range of parameters, from basic indicators like temperature and pH to complex biomarkers such as gastrointestinal health indicators, hormones, glucose levels, and drug concentrations, all in real time [5]. Such innovations open new opportunities for personalized, non-invasive health monitoring.

Keywords: *conductive ink, amperometric biosensors, glucose oxidase, stencil printing*

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Evaluation of the Biological Properties of a Multifunctional Natural Supplement for Liver Protection

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The liver plays a central role in detoxification and metabolism, but it is also highly vulnerable to inflammatory diseases such as hepatitis, cirrhosis, and non-alcoholic fatty liver disease (NAFLD) [1]. These conditions, often exacerbated by infections, represent a growing global health concern due to their increasing prevalence. Effective therapeutic strategies are urgently needed to address both the inflammation and the infectious triggers associated with liver dysfunction. Natural products have emerged as promising allies in this context, offering bioactive compounds capable of supporting liver health through anti-inflammatory, antioxidant, and antimicrobial activities [2]. Epavin, a dietary supplement by Erbenobili, combines a synergistic blend of plant extracts, including *Taraxacum officinale* (L.), *Silybum marianum*, *Peumus boldus* Molina, and *Cynara scolymus* L., formulated to support liver function. This study investigated the biological activities of Epavin, focusing on its antioxidant, anti-inflammatory, and antimicrobial properties. Furthermore, the protective effect of Epavin against heavy metal-induced toxicity has been assessed. Herein, the results will be discussed.

Keywords: *natural products, antioxidant, antimicrobial, anti-inflammatory.*

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H_2S releasing FPR2 agonists against neuroinflammation

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Neurodegenerative diseases such as Alzheimer's disease are strongly linked to neuroinflammatory processes. While physiologically this would be a protective response to harmful stimuli, protracted neuroinflammation causes oxidative stress and tissue damage, contributing to neurodegeneration and driving forward disease progression and symptoms[1].

In recent years, a significant amount of research has gone into finding anti-neuroinflammatory targets. Formyl Peptide Receptor 2 (FPR2), a G protein-coupled receptor expressed by the microglia, is one such target. FPR2 is interesting as it binds several ligands, eliciting pro-inflammatory or anti-inflammatory signaling depending on their structure[2].

Our group previously developed the ureidopropanamide class of FPR2 agonists [2]. In the present work, we show the introduction of H_2S releasing moieties into the ureidopropanamide scaffold. While a toxic gas at high doses, H_2S is physiologically produced in very low quantities as a result of cystein metabolism, and is a gasotransmitter involved in the inflammation of nervous activity and inflammation[3]. Thus, we synthesized thioureido and thioamide derivatives of our ureidopropanamide FPR2 agonists.

These compounds were assayed as FPR2 agonists, as well as H_2S releasers in HepG2, N9 and SH-SY5Y cells. Their neuroprotective activity was also assayed in primary mouse microglia, showing their promising profile as anti-neuroinflammatory compounds.

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Therapeutic Challenges in Pediatric Diffuse Intrinsic Pontine Glioma: Insights into the Structural Evolution of Human Protease ClpP Activators

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ONC201 analogues targeting the human mitochondrial protease ClpP are emerging as a pivotal therapeutic strategy for Diffuse Midline Gliomas, including the extremely aggressive pediatric **Diffuse Intrinsic Pontine Glioma** (DIPG).[1] ***h*ClpP** is highly expressed in gliomas as in other tumors, suggesting its potential as an agnostic therapeutic target. ONC201 induces hyperactivation of *h*ClpP, driving mitochondrial proteome degradation, enhancing stress response, and promoting apoptosis.[2] Despite the initial success rates, some DIPG patients developed resistance to ONC201, highlighting the need for new drug-like development. Medicinal chemistry efforts focused on synthesizing novel compounds with enhanced potency towards ***h*ClpP**. Novel tetrahydropyridopyrimidindiones as **THX6** shown efficacy in preclinical DIPG models by selectively disrupting mitochondrial homeostasis and impairing processes critical to tumor cell survival (Figure 1).[3] This presentation will discuss the design and synthesis of new *h*ClpP activators, their structural evolution and bio-pharmaceutical characterization, providing a better understanding of how to target mitochondrial vulnerabilities in cancer cells to promote therapeutic strategies for DIPG.

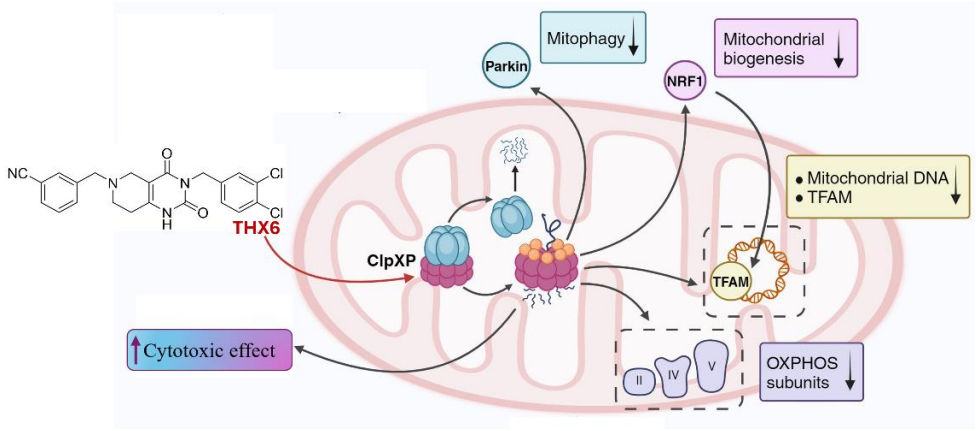

*Figure 1. Disrupted mitochondrial energy balance in tumor cells by **THX6**, driving them to death.*

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Keywords: *pediatric DIPG, ONC201, serine protease hClpP, tetrahydropyridopyrimidindiones*

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Rational optimization of the *N*-adamantyl-anthranil amide structural core for the developtment of new selective ligands for the Cannabinoid subtype 2 Receptor (CB2R)

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CB2R is a Gi-protein-coupled receptor (GPCR) which, together with CB1R, the endocannabinoids and the enzymes responsible for their synthesis and degradation, forms the endocannabinoid system (ECS). The expression of CB2R at the level of immune tissues, its over-expression, and up-regulation at the level of microglia cells in the CNS in pathological states, have led to questions about its role in inflammatory and neurodegenerative diseases. In 2023, we synthesized, evaluated, and published N-adamantyl-anthranil amide derivatives as CB2R selective ligands (Fig. 1B)[1]. We based our design on the proposed binding mode of the most potent CB2R antagonist AM10257, called "three-arm pose" (Fig. 1A). The best results in terms of affinity were observed in compounds presenting the phenyl ring or hydrogen on arm 1 and an alkyl chain with 5-carbon atoms as arm 2. The carboxy-adamantyl amide group as arm 3 was found to be critical for interaction with CB2R. We rationally explored a series of substitutions on the N-adamantyl-anthranil amide structural core as to assess any variations in affinity for CB2R. We also tested these synthetized compounds to evaluate their CB2R affinity and selectivity towards CB1R, obtaining interesting results. Compounds exhibiting the best pharmacodynamic profile in terms of CB2R affinity were also evaluated for the functional behavior and molecular docking simulations provided sound rationale.

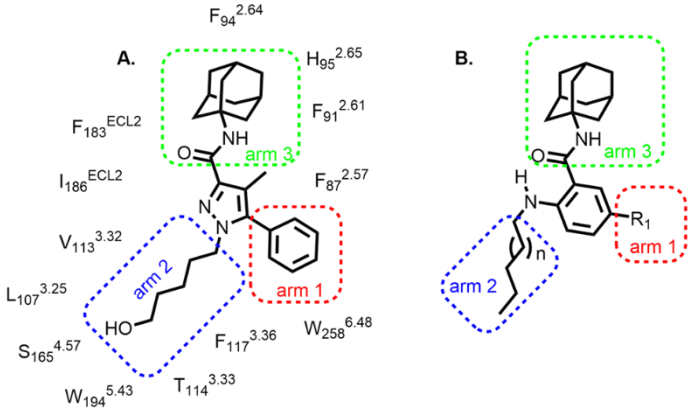

Figure 1: AM10257, CB2R antagonist (A), General structure of our N-adamantyl-anthranil amide derivatives (B).

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Pharmacokinetic Profiling and a Formulation Study on the FPR2 Agonist MR-39, a New Therapeutic Option for Autism Spectrum Disorder

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Autism Spectrum Disorder (ASD) is a group of heterogenous neurodevelopmental conditions characterized by social deficits, repetitive stereotyped behaviors, and neuroinflammation [1]. Abnormalities of the resolution of the inflammation (RoI) have been associated with ASD because decreased plasma levels of lipoxin A4 (LXA4), an endogenous mediator of RoI, have been reported in children affected by ASD [2]. LXA4 mediates its effect through the interaction with the N-Formyl Peptide Receptor 2 (FPR2), a G protein coupled receptor, that plays a key role in the inflammatory response and has emerged as a possible drug target for the treatment of chronic inflammatory diseases [3]. In a previous study, we reported that the administration of the FPR2 agonist MR-39 in BTBR mice strain and mice prenatally exposed to valproic acid (VPA), two animal models of ASD, reduced several inflammatory markers, stimulated neuronal plasticity, and improved social behaviour [4], thus proposing that promoting the resolution of inflammation through the activation of FPR2 might open new scenarios for the treatment of ASD. To date, there are no pharmacological approaches that can treat social deficits and stereotyped behaviors in ASD.

The aim of this study is to assess the developability potential of MR39 as clinical candidate for the treatment of ASD. To this end, an in-depth safety and pharmacokinetic profiling has been performed. In addition, considering the low aqueous solubility of MR39, different formulation strategies have been applied to address this issue.

We here report on MR39 profiling results and the potential as clinical candidate will be discussed.

Acknowledgements: this study was supported by Passion PoC Program, Piano Nazionale di Ripresa e Resilienza, Missione 1 "Digitalizzazione, innovazione competitività, cultura e turismo" – Componente 2 "Digitalizzazione, innovazione e competitività nel sistema produttivo" – Investimento 6 "Sistema della proprietà industriale" finanziato dall'Unione Europea – NextGenerationEU

Keywords: FPR2, Resolution of Inflammation, Autism Spectrum Disorders, Pharmacokinetic, Safety

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Development of ligands with high affinity for the pluripotent chaperon sigma1 (σ_1) as potential anti-SARS-CoV-2 agents

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The SARS-CoV-2 pandemic has highlighted the need to identify the virus's targets within the human body to disrupt mechanisms responsible for viral replication. An interesting interaction was observed between the viral protein Nsp6 and σ_1 receptor, a pluripotent chaperon involved in many physiological functions [1]. σ_1 Ligands with high affinity and selectivity were employed to support the antiviral activity mediated by σ_1 receptor. Compounds such as PB28 and its isoster F322 dispayed potent in vitro anti-SARS-CoV-2 activity (EC_{50} (PB28)= 0,299 µM; EC_{50} (F322)= 0,30 µM) (**Fig.1A**).

Background: Previous studies have shown that ligands with 4-methylpiperidine bound via an ethylene or propylene linker to a primary hydrophobic moiety such as tetralin, naphthalene or phenoxy rings[2,3,4], display high affinity and selectivity for σ_1 receptor.

Aim: σ_1-binding phenoxyalkylpiperidines, known for their drug-like properties and in vivo potency, were structurally modified to develop anti-SARS-CoV-2 agents. Modifications included i) substitutions on the benzene ring and replacement with isosteres, ii) change of the ethoxy linker into an aminoethyl one and iii) adjustments of the basic moiety with other cyclic structures (**Fig. 1B**).

Conclusions: Among the compounds obtained, there are subnanomolar affinity σ_1 ligands with notable selectivity towards the σ_2 subtype. The most promising ligands have been also investigated for their functional activity while the anti-SARS-CoV-2 in vitro assays are in progress.

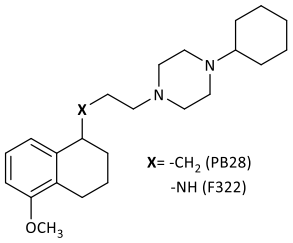
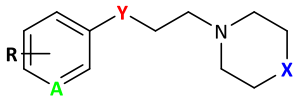


Figure 1A: PB28 and its derivative F322



R=-CF_3, -NO_2, -CH_3, -Cl, -F, -Br, -CN, -NH_2, -OH, -SO_2CH_3, -$NHSO_2CH_3$, -$CONH_2$, -OBn, -Ph, -OPh)
Y= O, NH
X= -NCH_3, -$CHCH_3$
A= -CH, N

Figure 2B: General structure of phenoxy and aniline -alkylpiperidines

This work was funded by Program PRIN of the Ministry of University and Reserach (PRIN 2022-2022Z3BBPE) and by Sigma1-Europe-European research network on sigma1 receptors CA23156.

Keywords: *σ_1 ligands, SARS-CoV-2, phenoxyalkylpiperidines and aniline -alkylpiperidines.*

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Flash Presentations

Photocatalytically enabled umpolung for the synthesis of hydroxyalkylkated and fluoroalkylated motifs

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Direct decarboxylative Giese reactions (DDGRs) represent a powerful yet underexploited tool in organic synthesis.[1] In the last couple of years, we have focused on the development of two new direct decarboxylative Giese strategies to install hydroxy-alkyl and monofluoro-alkyl fragments in complex molecular structures.[2] The main advantages of such approaches are represented by the simplicity of procedures, the use of inexpensive and often natural starting materials and the robustness of the protocols even when structurally complex reaction partners are involved. It is well known that hydroxy groups as well as fluorine atoms can significantly enhance the pharmaceutical properties of molecular structures. The introduction of a single hydroxyl group, in fact, can dramatically influence the drug−receptor binding affinity through the formation of an extensive hydrogen bond network.[3] Moreover, the -OH group can serve as a handle for further derivatizations. In the polar domain, hydroxyalkylations can be accomplished via different reaction pathways. However, retrosynthetically, the possibility to obtain γ-hydroxy substituted derivatives is precluded from polar mechanisms due to a polarity mismatch. α-hydroxyalkyl radicals have emerged as suitable intermediates to promote radical hydroxyalkylations.[4] The introduction of a fluorine atom, on the other hand, is of extreme interest to the pharmaceutical industry. Twelve of the fifty-five drugs approved by the FDA in 2023 contain at least one fluorine atom.[5] This piece of data is in line with the trend observed in the last decade, with approximately 20% of approved drugs being fluorinated. [6]Indeed, over the last two decades, it has been demonstrated that the introduction of a fluorine atom into the parent molecule can lead to therapeutic benefits through the modulation of lipophilicity, bioavailability, and metabolic stability. [7] We developed two photoredox-based direct decarboxylative reaction protocols which are compatible with various SOMOphiles. Furthermore, flow technology facilitates the scaling of these photochemical methodologies.[8,9]

Acknowledgements: We are grateful to Marilisa Pia Riganti for experimental support. We thank the European Commission – Horizon Europe Framework, project SusPharma grant agreement No 101057430 for financial support. M. C. acknowledges the Italian MUR for funding under the framework of the Action IV.6 PON R&I 2014–2020 – DM 1062. We acknowledge the CINECA award under the ISCRA initiative, for the availability of high performance computing resources and support (M. A., project code HP10CKZH2A).

Keywords: photocatalysis, fluorine, flow chemistry, alcohols

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A second life for e-waste: a catalyst from discarded capacitors active in the reduction of nitroarenes to anilines

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The aim of this study is to employ waste derived from electrical and electronic equipment (WEEE), such as capacitors from discarded printed circuit board (PCB), as catalysts in fine chemical reactions. The amount of electronic waste (e-waste) generated worldwide is constantly rising[1]. This type of waste contains potentially toxic and polluting substances, which pose a threat to human health and environment[2]. On the other hand, if properly managed, they become valuable resources thanks to their high content of critical raw materials (CRM)[1]. In this work the WEEE were initially ground to obtain a fine powder and some needles with a size less than 1 mm. Scanning Electron Microscopy (SEM) combined with Energy Dispersive X-Ray Analysis (EDX) and Thermogravimetric analysis (TGA) of the milled samples revealed the presence of potentially catalytic metals (Cu and Fe)[3] and plastic polymers. TGA results also allowed us to choose the suitable temperature for calcining the materials, carried out to eliminate the organic phase (plastic). The reductions of nitroarenes to their corresponding anilines were selected as a class of reactions to test the catalytic activity of the materials (cat-wire and cat-powder) obtained from multilayer ceramic capacitors after grounding and calcination. As benchmark reaction we used the reduction of nitrobenzene to aniline in water, at room temperature, with $NaBH_4$ as reducing agents. The magnetic catalyst, cat-wire, could be easily separated from the reaction mixture and recycled up to six times. Cat-wire was also active in the reduction of other substituted nitro compounds.

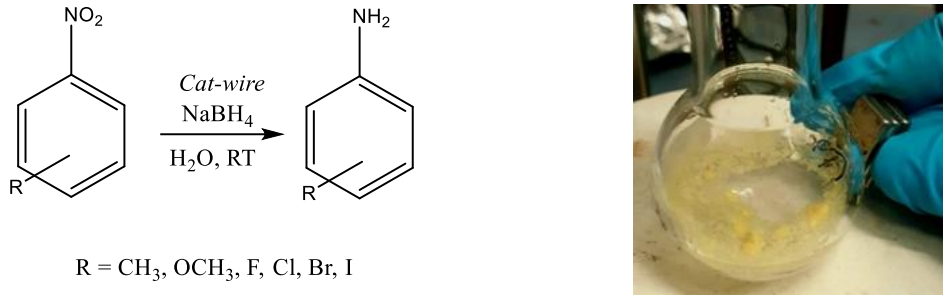

Figure 1: Reduction reaction of nitroarenes catalyzed by cat – wire and magnetic separation of cat-wire from mixture reaction.

Keywords: *catalyst from e-waste, Nitroarenes catalytic transfer hydrogenation, copper, iron*

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Study of eco-sustainable methods for reducing the organic fraction responsible for Chemical Oxygen Demand (COD) in wastewater from industrial plants

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The Fenton reaction is an advanced oxidation process (AOP) that uses the interaction between hydrogen peroxide (H_2O_2) and iron-based catalysts, typically iron(II) ions (Fe^{2+}), to generate highly reactive hydroxyl radicals ($\cdot OH$)[1-2]. These radicals effectively degrade complex organic compounds, making the Fenton reaction a promising technology for treating organic pollutants in wastewater and contaminated soils. Its ability to reduce Chemical Oxygen Demand (COD) and convert contaminants into less toxic byproducts highlights its environmental importance[1].

A major incentive for using the Fenton reaction is compliance with environmental regulations, such as the European Union Water Framework Directive (Directive 2000/60/EC) and REACH Regulation, which set strict COD limits for wastewater discharge, typically between 25 and 125 mg/L. Exceeding these limits indicates excessive organic load, threatening water quality and ecosystems, and underscores the need for efficient treatment technologies.

This research aims to improve the Fenton reaction's efficiency and sustainability by focusing on heterogeneous catalysis and introducing recycled metal-based catalysts derived from metallic scraps. Materials like metallic components contain valuable metals (e.g., iron, copper, nickel) that can be recovered and repurposed as catalysts (Figure 1). This approach reduces costs while supporting a circular economy by transforming wastes into valuable resources[3].

Using recycled materials offers significant environmental benefits, reducing dependence on mining and providing a sustainable solution for metallic waste management. Optimizing parameters such as H_2O_2 dosage, system pH, and catalyst concentration can further enhance the process. These advancements make the Fenton reaction an efficient and environmentally responsible method for pollutant removal.

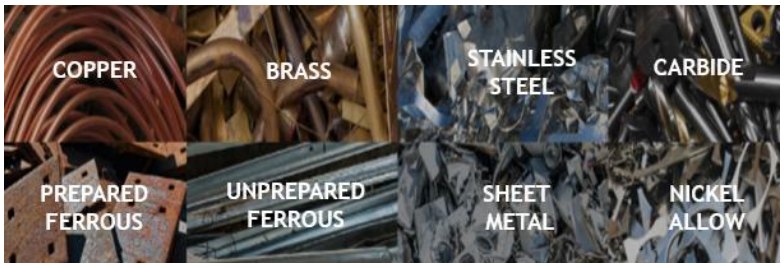

Figure 1 : Common metallic scraps

Keywords: *COD, Metallic scrap, Water treatment*

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Livestockfarm WasteWater (LWW) treatment through an advanced approach: the application of electrochemical oxidation

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The wastewater from livestock farms is typically rich in ammonium nitrogen, which is transformed into nitrate by aerobic bacteria spontaneously present in the soil when it is spread on the fields. Nitrate is highly soluble in water and leaches into the soil, reaching surface water and groundwater, leading to human, environmental, economic and social risks. Therefore, removing ammonium nitrogen is pivotal. In addition, livestock wastewater is also rich in organic compounds (measured as Total Organic Carbon – TOC), which must be removed too. The abatement of these compounds was investigated during the experimental activity. Their removal was carried out through an advanced approach consisting of electrochemical oxidation. Electrochemical treatment is a chemical transformation of compounds with an external electrical circuit. Nitrogen compounds are brought to complete oxidation when they reach the gaseous nitrogen, limiting nitrate production below the regulatory limit, while organic compounds, when they reach the completely oxidated, are transformed into carbon dioxide. Efficient wastewater treatments constitute crucial strategies for its proper management. The removal of nitrogen compounds and TOC was investigated by using a pioneering plate reactor equipped with titanium oxides and iridium electrodes (surface: 20x22.5 cm^2). A current density of 11.1 A m^{-2} was applied. The initial concentration of total nitrogen (TN), ammonia (NH_4^+) and TOC was 47 mg L^{-1}, 22.8 mg L^{-1} and 392 mg L^{-1}, respectively. The initial pH of the solution was 8. The removal efficiency as a function of the time is reported in Figure 1, in which nitrate formation (NO_3^-) is also included. As shown, with the operative conditions tested after 180 minutes of treatment, removals of 27.5%, 58.9% and 35.1% for TN, NH_4^+ and TOC were achieved, respectively. The removal of 58.9% for NH_4^+ allows the achievement of the concentration of 9.3 mg L^{-1}, below the Italian regulatory limit for the discharge in superficial water (15 mg L^{-1} – D.Lgs 152/2006). In addition, a concentration of 1.3 mg L^{-1} of NO_3^- was measured, which is below the Italian regulatory limit for the discharge in superficial water (20 mg L^{-1} – D.Lgs 152/2006).

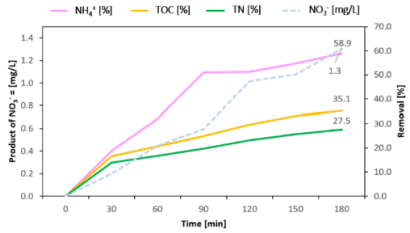

Figure 1: TN, NH_4^+ and TOC abatment, and NO_3^- formation

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***Keywords:** Electrochemical, Nitrogen Removal, Environmental Pollution, Advanced reactor*

Green solvents as an alternative, sustainable practice for the recovery of phenolic compounds in grape pomace

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The large amount of agro-industrial wastes, generated by massive agricultural production to respond to the gradual increase in global population, are recognized as one of major causes of the environmental pollution worldwide [1]. For this reason, it is important to find sustainable strategies aimed on reusing these by-products, exploiting their potential as alternative sources of health beneficial bioactive molecules[1].
In the first part of the project, Cabernet Sauvignon and Petit Verdot grape pomaces collected in 2023 were characterized and used to perform solid-liquid extractions employing, as liquid green extracting phases, the so-called Deep Eutectic Solvents (DESs) and hydroalcoholic solutions as reference. The chemical characterization performed with a newly developed HPLC-DAD method on both fresh and dried grape pomaces, provided the phenolic compounds' profile. In all thirty-six samples analysed, up to eight out to thirteen phenolic compounds taken as standards (gallic acid, coumaric acid, syringic acid, caffeic acid, catechin, rutin, quercetin and kaempferol galactoside) were detected with a maximum concentration of a single analyte determined in a single sample of 0.49 µg/g (quercetin). Two different DESs were selected as the best ones for fresh and dried grape pomaces, and will be used for the further optimization experiments. Then, the DPPH radical photometric assay was chosen to determine the relative antioxidant activity of the extracts. The encouraging results displayed an activity up to 14.9 mM Gallic Acid Equivalents. New in vitro bioassays and food fortification experiments are now planned. Ultimately, the possible use of the extracts in feed supplementation will also be evaluated.

Acknowledgements: V.R. fellowship was funded by Unione Europea -Next Generation EU. M.U.R., D.M. 02/03/2023, N. 118. Titolo Progetto: Soluzioni sostenibili per la produzione di nuovi integratori ottenuti a partire da scarti dell'industria alimentare.

Keywords: *Grape pomace, sustainability, nutraceuticals, Deep Eutectic Solvents (DESs).*

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Integrating epoxidation and high-resolution mass spectrometry to unravel the complex profile of Boswellic acids in Boswellia serrata Gum Resin Extract

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The chemical characterization of natural products is often a complex task that demands powerful analytical techniques. Liquid chromatography with high-resolution tandem mass spectrometry (HRMS/MS) is often employed, yet it can face hard challenges when isomeric species are present, and reference standards are lacking. In such cases, the confidence level in compound identification can be significantly improved by the collection of orthogonal information on target analytes. In this work, 23 key compounds in *Boswellia serrata* extract (BSE), 12 of which correspond to boswellic acids (BAs) and 11 to triterpenoidic acid isomers, were identified by combining RPLC followed by serial UV and ESI(-)-FTMS and FTMS/MS detections with the evaluation of the reactivity towards C=C bond epoxidation with meta-chloroperoxybenzoic acid (m-CPBA), proposed as a fast chemical tool to gather information about C=C bond steric hindrance, a key structural feature of BAs and related compounds. BAs are a class of pentacyclic triterpenoids that make up 25% of the lipophilic component of *Boswellia serrata* gum resin, which is also known as frankincense or olibanum [1,2]. Historically, frankincense has been widely used in religious and cultural ceremonies as an ingredient of traditional medicines [3]. BAs are recognized as the primary bioactive components of frankincense due to their therapeutic effectiveness against chronic inflammatory diseases [1,2].

The interpretation of MS/MS based on higher-energy collision-induced dissociation (HCD) unveiled new fragmentation pathways, providing important structural details on target analytes. The integrated approach developed during this study[4] might pave the way for a deeper understanding of the BSE bioactive properties. Moreover, it can be considered an example of a more general strategy for the analysis of complex mixtures of natural compounds including also isomeric species.

Keywords: *Boswellic acids, epoxidation, high-resolution tandem mass spectrometry, natural products.*

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Development of a chromatography free method based on DART-Triple Quadrupole mass spectrometry for targeting safflower and turmeric as adulterants in saffron

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Direct analysis in real time-mass spectrometry (DART-MS) is a rapid and accurate analytical technique that does not require extensive sample preparation and has been exploited in food analysis for the detection of contaminants including pesticides, mycotoxins and in forensics[1,2]. Saffron is a valuable spice derived from *Crocus sativus* stigmas and due to the high costs has been the main target of many fraudulent actions. For saffron quality assessment the ISO 3632-1:2011 is applied, which relies on spectrophotometric and chromatographic analysis. Despite the traditional methods requiring complex and long protocols, new robust and fast methods are urgently demanded in order to detect any possible adulterant in saffron at a concentration lower than 20% this last representing the lowest level that can be detected by conventional methodologies[3].

In this note we describe the development of a fast, robust, and high throughput screening method for safflower and turmeric detection as adulterants in safflower.

The study explores the potential of DART-MS combined with targeted Multiple Reaction Monitoring (MRM) on a DART-EVOQ triple quadrupole mass spectrometer for the detection and quantificationof safflower and turmeric in saffron at the lowest level of 5%. Safflower and turmeric powders (n=2each) and saffron pure or adulterated with safflower (5-10-20%, n=2 each) and turmeric (5-10-20%,n=2 each) were briefly extracted with a mixture of water/solvent and analyzed by DART-MS withoutfurther preparation. Calibration curves for each adulterant were created by mixing saffron and adulterants extracts at varying inclusion levels (covering the range 10-70%). By running full scan and Product Ion Scan experiments some potential markers were identified and after selection of the best transitions for each marker upon optimization of the collision energy, MRM experiments were carried out tailored to perform quantitative analysis. Specific markers along with their main fragments for safflower 116.2>70.1; 446.2>116.2 m/z and for turmeric 368.9>116.2; 339>116.2 m/zwere confirmed as suitable markers for detecting adulteration. Calibration curves showed a strong correlation, further improved with the introduction of an internal standard, confirming the successful development of a rapid, high-throughput method for detection of traces of safflower andturmeric in saffron ad. Summarizing a quick DART – MS/MS target method was developed on the new EVOQ triple Quadrupole mass spectrometer capable of detecting the addition of tiny amountsof safflower and turmeric adulterating saffron at the lowest level of 5% through the detection of two markers and relative transitions.

Acknowledgements: Bruker Corporation is kindly acknowledged for supporting this research.

Keywords: *DART-MS, targeted analysis, saffron authenticity, metabolite analysis*

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Investigating the effect of different cooking treatments on the formation of polycyclic aromatic hydrocarbons in meats by means of GC-MS/MS

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Polycyclic Aromatic Hydrocarbons (PAHs) is a group of about 200 organic compounds formed by two or more aromatic condensed rings, considered as significant food processing contaminants, characterized by mutagenic and carcinogenic properties. In particular, meat cooking can lead to the formation of these harmful compounds. The maximum residue levels for the sum of 4 PAHs and for benzo[a]pyrene (BaP) in food products are established in Europe by the Regulation (EU) No. 915/2023.

In this study, six different cooking treatments were tested on four different types of meat, such as loin, neck, chicken and bovine hamburger. Four of these treatments were also carried out prolonging the cooking time to verify PAHs possible increase. The analytical determination of 4 PAHs (benzo[a]anthracene (BaA), chrysene (Chry), benzo[b]fluoranthene (BbF) and benzo[a]pyrene) was obtained using a fully validated and accredited method by QuEChERs dispersive solid phase extraction coupled to GC-MS/MS[1]. A study on the chromatographic separation of benzofluoranthene isomers was also carried out.

The overall evaluations have highlighted that some characteristics of various cooking techniques can influence the formation of PAHs, particularly cooking time and oil use.

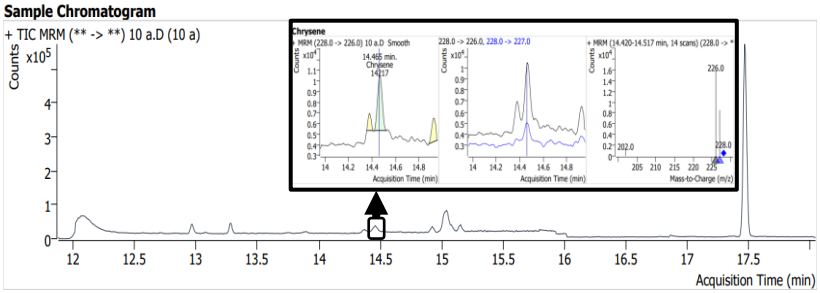

Figure 1: Chromatogram example where chrysene was detected after cooking

Acknowledgements: This study was supported by the Italian Ministry of Health (Rome, Italy) who financed the Research Project code IZSPB 06/21 RC.

Keywords: *PAHs, cooking, meat, GC-MS/MS*

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Separation and analysis of the cis- enantiomers of Cypermethrin based on QuEChERS and GC-MS/MS analysis

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The presence of pesticide residues in food is a significant topic in food safety worldwide. In this regard, the European Commission provides continuous updates of the legislation regarding all aspects related to the possible presence of pesticide residues in food, with particular attention to the definition of specific maximum residue limit (MRL) for each pesticide. Although pesticides have found widespread application and have played a significant role in the steady increase in agricultural and animal production, the risks they have brought with them to food safety and human health have increasingly become the focus of global attention [1]. α-Cypermethrin is an insecticide from the pyrethroid family of chemicals and it is approved as a biocidal active ingredient pursuant to European Regulation [2]. This pesticide is toxic if ingested and may cause organ damage through prolonged or repeated exposure causing severe respiratory irritation. The α-Cypermethrin formula, used in agriculture, is a racemic mixture of two isomers, i.e. 1R cis S and 1S cis R, of the four cis isomers of Cypermethrin [3]. In consideration of the greater toxicity of α-Cypermethrin compared to other isomers, it is necessary to lower the MRL value for a conservative approach that safeguards the health of the consumer, considering a worst-case scenario where all the quantity of residue found referred only to the α-Cypermethrin isomer. Our laboratory participated in the Proficiency Test EUPT-FV26 organized by EU Reference Laboratories for Residues of Pesticides. The EUPT-FV26 test item, banana, was spiked with technical Cypermethrin, so it contained all the isomers. Therefore, the formal evaluation of Cypermethrin was made on the sum of isomers. There was a problem because of the 175 participants, only 59 reported specific results for α-Cypermethrin. Concentrations reported ranged between 0.012 and 0.136 mg/kg, with a robust mean value of 0.057 mg/kg and CV % is 69%. Such a high dispersion of the results evidences the need to solve the analytical difficulties of its analysis. The technical mixture of Cypermethrin has 4 pairs of enantiomers, resulting in 4 chromatographic peaks. The latter two peaks tend to co-elute. In the adapted EURL-FV multiresidue method, α-Cypermethrin elutes as the third peak of the set. In certain conditions, the isomerization of α-Cypermethrin into a different enantiomeric pair has been observed. This process occurs through the substitution of the cyano moiety, which then returns to the original molecule with the opposite configuration. The resulting products correspond to the only pair that is not included under any of the remaining isomer definition, which is the first peak to elute. In this work, a validated multi-residual analytical method by gas-chromatography and tandem mass spectrometry was used to separate the Cypermethrin isomers by resolving the coelution of these two peaks. In this way, we can separate the four Cypermethrin isomers and thus be ready for the new European requests for official check analyses and monitoring studies, required for multi-residue analysis at trace levels.

Acknowledgements:The participation is supported by the Ministero della Salute with Research Project RC IZSPB 05/2023.

***Keywords**: Cypermethrin, GC-MS/MS, Proficiency test, QuEChERS*

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Alkaline Phosphatase Inhibition on Gold Nanocoral Electrodes for the Ultrasensitive Detection of 2,4-Dichlorophenoxyacetic Acid

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2,4-Dichlorophenoxyacetic acid (2,4-D) is an herbicide used to control broadleaf weeds in cereal crops. However, the presence of 2,4-D residues in food and the environment poses serious health risks to humans and animals. Regulatory agencies, such as the US Environmental Protection Agency (EPA) and the European Commission, have set stringent limits on 2,4-D concentrations in food and water. This underscores the need for effective and rapid methods to detect 2,4-D residues. Traditional analytical techniques, while highly sensitive, are often expensive, require specialized expertise, and are not suitable for real-time, in situ monitoring. As a result, there has been growing interest in developing biosensors that offer rapid, cost-effective, and portable detection for environmental contaminants. Enzyme inhibition-based biosensors, in particular, have emerged as promising tools for continuous environmental monitoring. These biosensors exploit the kinetics of enzyme inhibition to detect contaminants such as 2,4-D. Although previous studies have developed ALP-based biosensors for detecting 2,4-D, challenges such as enzyme instability remain.

This study reports the development of an ultrasensitive enzyme inhibition-based biosensor for 2,4-D detection, utilizing alkaline phosphatase (ALP) immobilized on a photo-crosslinked poly(vinyl alcohol) matrix functionalized with N-methyl-4(4'-formylstyryl)pyridinium (PVA-SbQ), supported by highly porous gold nanocoral (hPGNC) electrodes. After electrochemical and morphological characterization, the PVA-SbQ/ALP/hPGNC electrode was tested for inhibition studies using ascorbate 2-phosphate (A2P) as the substrate. The sensor demonstrated a preparation and sensing time of approximately 45 minutes, with amperometric measurements providing reliable results in just 5 minutes. The biosensor exhibited a linear detection range from 0.002 to 22 ppt, with a sensitivity of 0.121 ± 0.006 ppt^{-1} (RSD = 4.9%, R^2 = 0.996, N = 6) and a limit of detection (LoD) of 0.7 ppq, 7–8 orders of magnitude below regulatory thresholds in Europe and the USA. The biosensor was validated using spiked wheat leaf extract samples, showing excellent recovery (96%) and reproducibility (RSD < 9.8%). Additionally, it demonstrated robust operational and storage stability, retaining 84% and 94% of its initial response, respectively. These findings highlight the potential of the PVA-SbQ/ALP/hPGNC biosensor for real-time, on-site 2,4-D monitoring in agricultural settings, with prospects for integration with artificial intelligence systems for advanced diagnostics.

Keywords: *Biosensors, analytical chemistry, 2,4-D detection, enzymatic inhibition, highly porous gold*

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Diatom Microrobots as effective and biodegradable agents against water-borne pollution

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Bio-based functional materials are currently being used in a variety of applications, from sensing to catalysis [1], with bio-inspired and biomimetic polymers holding great promise due to their chemical diversity and tuneability. Polydopamine (PDA) is a biocompatible and bio-inspired polymer, that can be easily synthetized via spontaneous oxidative polymerization of dopamine in water. Even though the structure of PDA has not been yet fully described, it exhibits interesting features like adhesive and entrapping properties and tuneable porosity [2]. PDA has been used in combination with living microorganisms, taking advatngae of its adhesive and entrapping properties [3]. Moreover, the presence of specific chemical groups in PDA, like charged groups and aromatic rings, allows it to interact and trap specific compounds, such as polyaromatic or polychlorinated hydrocarbons [4]. This work aims to optimize the fabrication of a biocompatible PDA-based coating onto living diatoms, explore the decoration with additional functional elements (nanoparticles, enzymes, etc), and test their performance as biohybrid functional materials. Their catalytic activity has been tested under repetitive tests of recycle and in long-term experiments, with promising results. These biohybrid microrobots have potential applications in bioremediation and biomedicine.

Acknowledgements: This work was supported by H2020-MSCA-ITN-2019 project 860125-BEEP (Bioinspired and bionic materials for enhanced photosynthesis).

Keywords: Diatoms, Bioremediation, Polydopamine, Microrobots

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Development of potent mitochondrial *h*ClpP activators for cancer therapy through a process of structural simplification

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Human caseinolytic protease P (*h*ClpP) is a serine protease found in the mitochondrial matrix, playing a crucial role in mitochondrial proteostasis. Together with the AAA+ unfoldase protein ClpX, *h*ClpP forms the *h*ClpXP complex, responsible for facilitating the turnover of misfolded or damaged proteins, thereby preventing their accumulation and ensuring cellular function. *h*ClpP expression is upregulated in various solid tumors, including lung, stomach, liver, thyroid, bladder, breast, ovary, prostate, testis, and brain tumors. As a result, chemical modulators of *h*ClpP activity have potential as anticancer agents. *h*ClpP activators, such as imipridones, acyldepsipeptides (ADEP), and oxadiazonocarboxyamides, induce the dissociation of ClpX from ClpXP, and ClpP maintains the proteolytic activity. Among these, imipridones, particularly ONC201, have been the most extensively studied. Using *in silico* methods, a new scaffold featuring "tetrahydropyridopyrimidione" (THPPD) was identified, and its derivatives were found to be 50-100 times more potent activators of *h*ClpP than ONC201. Simplifying this scaffold to 1,4-dibenzylpiperazine-2-one derivatives (DA series) we have proven that the activation of *h*ClpP is affected by the electronic properties of substituents on the aromatic rings (R^1 and R^2) and by the introduction of an endocyclic carbonyl into the piperazine core ring. These modifications enhanced the proteolytic activity of *h*ClpP, with compounds exhibiting increased activation potency. Our structure-activity relationship study provides valuable insights to design more potent *h*ClpP activators.

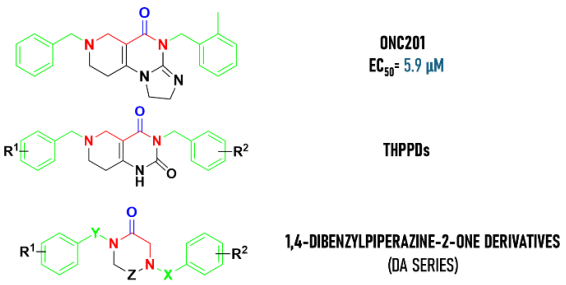

Figure 1: Structural evolution of ONC201 to the new piperazine derivatives.

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Keywords: *mitochondrial human ClpP, drug discovery, cancer therapy.*

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Development of fluorescent ligands: greener and safer tools useful to drug discovery

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Fluorescence imaging is a technique useful to investigate the mechanisms of various proteins, with multiple applications. From a greener and safer perspective, it serves as a valuable alternative to the traditional use of radioligands. This work fits within this context, aiming to explore and study the mechanism of action of sigma-1 receptors (S1R) and CB-2 receptors (CB2-R), promising therapeutic targets with unclear mechanisms of action. S1R, a subtype of sigma receptors, is a pluripotent chaperone involved in a plethora of pathologies such as CNS diseases, cancer and neuropathic pain.[1] Similarly, CB2R, part of the endocannabinoid receptor family, operates via G protein coupling and plays crucial role in inflammatory, immune, and neurological pathways.

In developing S1R ligands, we focused on designing fluorescent compounds based on **L13**, a lead compound with sub-nanomolar affinity for S1R[1]. We modified L13's phenoxyalkylpiperidine structure by attaching various fluorescent tags at the para position of the benzene ring using different alkyl linkers. The resulting compounds displayed high affinity for S1R with fluorescence emission from green to red regions of the light spectrum. (Figure 1A)

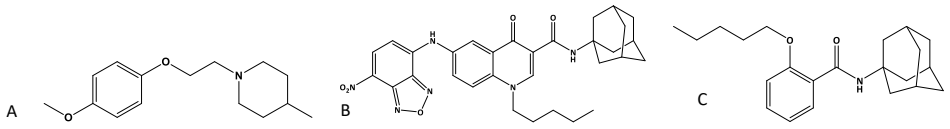

Figure 1. Lead compounds scaffolds: L13 (A); VM7 (B), FI8 (C)

As for CB2R ligands, we focused on synthesizing molecules with a 4-oxoquinolinone scaffold or a salicylamide one, based on the optimal pharmacodynamic profile of the green-fluorescent **VM7**[2] or on the high-affinity CB2R agonist **FI8** (Figure 1 B, C). With the aim to obtain red emitting VM7 analogues, and fluorescent derivatives of **FI8**[3] we are investigating different spacers between the two pharmacophores and diverse fluorescent tags. The most promising S1R and CB2R ligands will undergo further evaluation through different fluorescence-based biological assays to be validated as tools useful to drug discovery.

This work was supported by PNRR - Missione 4, componente 2 "Dalla Ricerca all'Impresa" - Investimento 4.1 "Estensione del numero di dottorati di ricerca e dottorati innovativi per la pubblica amministrazione e il patrimonio culturale" (D.M.N. 118)

Keywords: Fluorescence, sigma-1 receptor, CB-2 receptor.

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Assessing the Antitumor Potential of Monofunctional Platinum(II)-Nucleoside Complexes: Synthesis, Characterization, and Cytotoxicity Studies of cis-[Pt(NH3)2(Guo/dGuo)X] (X = Cl, Br, I)

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Following the successful use of cisplatin in cancer treatment, there has been a significant focus on investigating metal-based compounds with potential antitumor properties. Despite the effectiveness of approved platinum drugs against various types of cancer, their lack of selectivity towards tumor cells and the development of drug resistance makes necessary the search for new platinum-based antitumor agents. Among these, Pt(II)-nucleoside complexes have shown promise as antimetabolites for anticancer therapy [1]. Specifically, complexes of the type *cis*-$[Pt(NH_3)_2(Am)Cl]^+$ (Am = heterocyclic imine derived from pyridine, pyrimidine, purine, piperidine, or saturated amine) have demonstrated high stability and solubility in aqueous media, as well as interesting *in vitro* and *in vivo* antitumor potential against various tumors, including sarcoma and leukemia [2]. Recently, we synthesized six complexes of the type *cis*-$[Pt(NH3)_2(Am)X]^+$, where Am = guanosine (Guo, **a**) or 2'-deoxy-guanosine (d-Guo, **b**) and X = Cl (**1**), Br (**2**), or I (**3**). These cationic platinum species were characterized using NMR spectrometry and their potential antiproliferative activity was evaluated in different cancer cell lines (Caki-1, HeLa, MCF-7, Raji, ZL-34) and compared with their cytotoxicity in a normal cell line (HK-2). Our findings suggest that halogen substitution may be a simple method to alter the cytotoxic and biological activities of these complexes while maintaining their molecular structure.

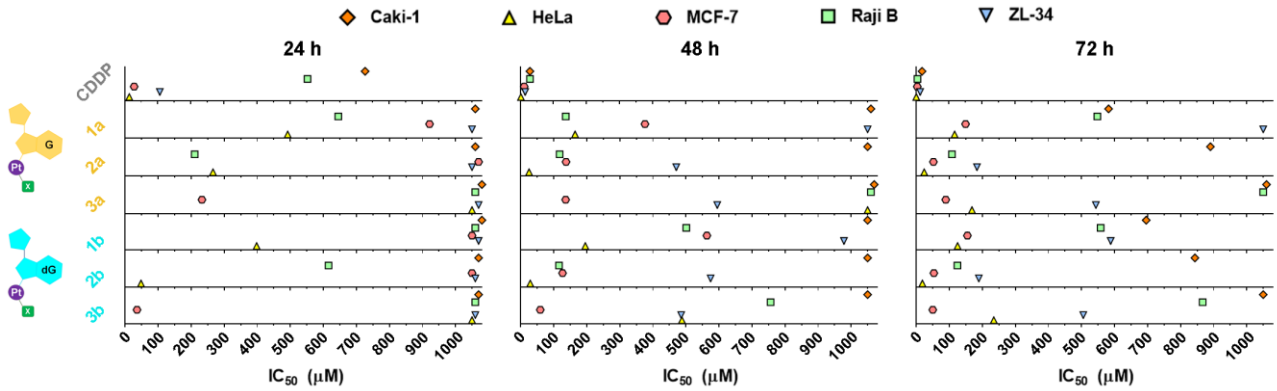

Figure 1: IC50 values determined for five cancer cell lines (Caki-1, HeLa, MCF-7, Raji, ZL-34) after exposure to cisplatin (CDDP) and Pt(II) nucleoside complexes (1a-3a; 1b-3b) for 24, 48 and 72 h.

Acknowledgements: The authors acknowledge the University of Salento (Italy) and the "BIO-D" project "Sviluppo di Biomarcatori Diagnostici per la medicina di precisione e la terapia personalizzata" (ARS01_00876) for financial support.

Keywords: *Cisplatin, Metal-based compounds, Antitumor agents, Pt(II)-nucleoside complexes.*

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Composite electrodes for enhanced ozone-based water treatment: development and characterization of nanostructured titanium substrates

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Ozone-based processes are frequently employed to treat water contaminated with microorganisms and harmful organic and inorganic residues. Despite the high redox potential of ozone, there is frequently a low degradation rate and negligible mineralization of organic compounds. To improve the performance of this process, the combination with electrochemical methods, has recently been proposed. In this way, powerful oxidizing species are generated in situ without the need for the addition of further reagents. However, the development of the procedure is partly slowed down by the poor resistance of commercial electrodes which, although exposed to relatively low current densities, work in extremely difficult conditions. This project aims at the development of a composite electrode based on titanium, which provides a robust, corrosion-resistant substrate and a metal redox active material to improve the electrochemical reduction of ozone.

To maximize the active surface, the metal was deposited as nanoparticulated material. Particular attention was paid to the characterization of the initial NPs growth phase to better correlate synthesis parameters and material performance. In addition, the titanium surface was etched with acids and bases to create a rough, nanostructured surface which can influence the deposited NPs' morphology and density. The impact of these surface modifications was evaluated and compared with untreated substrates.

The materials were characterised using various techniques, including scanning electron microscopy (SEM), X-ray diffraction (XRD), contact angle measurements, electrochemical impedance spectroscopy (EIS) and cyclic voltammetry.

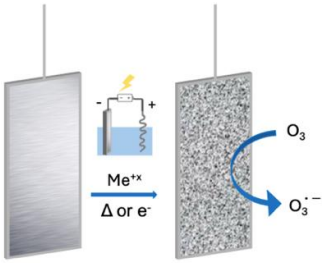

Figure 1: Electrode construction and operation

Keywords: *Ti surface modification, electrodeposited Me^{+} particles, ozone-based water treatment*

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Pectin/Gellan gum hydrogel films embedded with saffron by-products: a promising strategy for wound healing

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During the processing of saffron as a spice, several floral bioresidues are generated, including tepals and stamens. Recent studies reported that both of these floral parts can represent a good source of bioactive molecules, mainly polyphenols.[1] In this study, hydrogel films based on Gellan gum (GG) and Pectin (Pec), with tartaric acid and $CaCl_2$ used as cross-linking and glycerol as plasticizing agent, have been used as a carrier for *Crocus sativus* tepal extract (CSE). The aim is producing a composite applicable for the regeneration and healing of cutaneous wounds, exploiting the anti-inflammatory and antioxidant properties of CSE obtained by saffron by-products. The good adaptability to skin morphology, elasticity and biocompatibility given by the polysaccharides blend, allow to the hydrogel films good carrier ability for CSE components. The excellent CSE antioxidant properties provide an effective strategy to fight significant cellular oxidative stress typical of skin wounds, allowing healing of damaged cellular tissues.[2,3] The films were subjected to chemical-physical characterization by FTIR-ATR, XPS, TGA and DSC. Evaluation of water-uptake and water holding capacity were monitored in simulated wound fluid and PBS. The CSE and CSE-loaded films' total polyphenols content, and the antioxidant activity by ABTS and DPPH assays, were also evaluated. *In vitro* biological performances of the proposed materials were tested on human normal dermal fibroblasts (NhDFs) and on an immortalized keratinocyte cell line (HaCaT), demonstrating good cytocompatibility and *in vitro* tests on senescent cells confirm the possible application to enhance the healing of chronic wounds.

Figure 1: From left to right: 1.6:0.4, 1:1, 0.4:1.6 Pec:GG/CSE films

Keywords: *Hydrogel, Pectin, Gellan gum, saffron.*

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Advanced x-ray scattering techniques for structural characterization of antibacterial nanostructured biomaterials

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X-ray scattering techniques are suitable for studying various types of materials in different physical states (liquid, gel, solid). These techniques typically investigate crystalline phases, domain sizes, shapes, and textures. The crystalline components are mainly studied by Wide Angle X-ray Scattering (**WAXS**), providing information on the crystallinity and crystalline phases, as well as on possible texture1. Transmission and reflection geometries are successfully employed, to exploit lateral spatial resolution and surface sensitivity, taking advantage of microdiffraction/scanning microscopy and grazing incidence options (**GISAXS/GIWAXS**), respectively. The Institute of Crystallography of CNR (CNR-IC) in Bari is equipped with two complementary setups: the XMI-Lab (Figure 1a), which couples a Rigaku Fr-E+ SuperBright Cu micro-source to a SMAX3000 SAXS/WAXS camera[1], and a Xenocs Xeuss 3.0 HR, equipped with a Motorized Dual source module that includes Excillum Ga Metal jet and Cu Genix3D micro-sources[2]. The high brilliance available at XMI-L@b has been successfully applied to the study of free-standing nano/bio-materials. Data are analyzed by using the in-house developed software SUNBIM[3]. CaP-based Antibacterial Nanostructured Surfaces were studied through X-ray scattering in transmission and grazing incidence reflection geometries (Figure 1b) to probe structure and texture of all material layers from the amorphous CaP substrate to the intermediate Hydroxyapatite crystallization layer, up to the crystalline nanoneedles on the top surface[4].

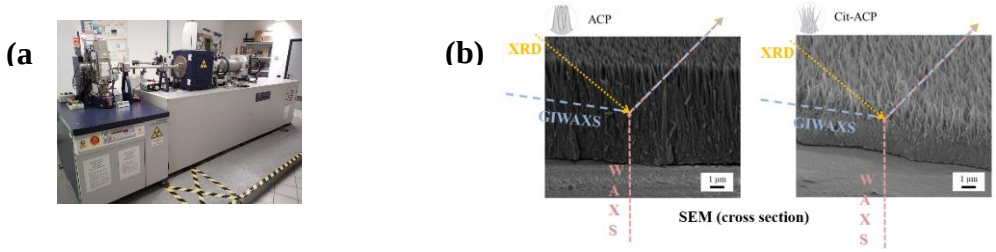

Figure 1. a) Rigaku Fr-E+ SuperBright rotating copper anode microsource for scanning SAXS/WAXS and (GI)SAXS/(GI)WAXS; b) Cross-section SEM of the CaP-based nano-biomaterials with indications of the reflection (GIWAXS and XRD) and transmission (WAXS) X-Ray scattering geometries.

Acknowledgements: This work was supported by the research project "Potentiating the Italian Capacity for Structural Biology Services in Instruct-ERIC", acronym "ITACA.SB" (Project No. IR0000009, CUP B53C22001790006), funded by the European Union's NextGenerationEU under the MUR call 3264/2021 PNRR M4/C2/L3.1.1/

Key words: *waxs, giwaxs, xrd, nano-biomaterials.*

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Chemical Recycling of Waste Polyolefins via Catalytic Hydroconversion

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Plastics have become the most widely produced man-made material. By 2015, an estimated 6,300 million metric tons of plastic waste had been generated, with only 9% recycled, 12% incinerated, and a staggering 79% accumulating in landfills or the environment. If current trends persist, approximately 12,000 million metric tons of plastic waste could accumulate in landfills or nature by 2050[1]. The extensive production of common polyolefins, such as polyethylene (PE) and polypropylene (PP), coupled with their low cost and widespread use in short-term applications, has created a critical challenge for waste management. Currently, only a small fraction of these materials is mechanically recycled, while the majority is either incinerated, landfilled, or escapes into the environment. Given their high energy content, there is increasing interest in recovering their chemical value and promoting more sustainable end-of-life practices[2]. This project aligns with these efforts, aiming to raise scientific and public awareness about the catalytic upcycling of waste polyethylene into valuable liquid alkanes. Thermochemical methods, such as pyrolysis and thermal cracking, enable the breakdown of polyolefins by cleaving the robust C−C bonds in PE, yielding small molecules that can be used as fuel. However, these methods are energy-intensive and face challenges in controlling product selectivity. By contrast, C−C bond dissociation through hydroconversion offers a more targeted approach, enabling the depolymerization of polyolefins into liquid alkanes within specific molecular weight ranges[3]. In this study, the hydroconversion of polyolefins was investigated using two types of ruthenium-based catalysts: monofunctional Ru/C, which primarily promotes hydrogenolysis, and bifunctional Ru/Al_2O_3, which facilitates hydrocracking. Results show that the conversion of polyethylene increases progressively with reaction time for both Ru/C and Ru/Al_2O_3 catalysts. Among the catalysts evaluated, Ru/Al_2O_3 exhibits significantly higher conversion rates compared to Ru/C. This superior performance is attributed to the enhanced catalytic activity of Ru/Al_2O_3, which efficiently facilitates hydrocracking reactions. Moreover, the Ru/Al_2O_3 catalyst consistently yields a higher fraction of hydrocarbons in the C_5–C_{20} range, the target product range for our application. This highlights its capability to promote selective hydrocracking, breaking down the polymer chains into desirable product fractions. The results underscore the efficiency of Ru/Al_2O_3 in producing valuable hydrocarbons, making it a more suitable catalyst for polyethylene hydroconversion processes.

Keywords: *polyolefins, catalyst, hydroconversion, fuels*

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Reactive behaviour of Platinum(II) salts with ethylenediamine in sustainable water-choline chloride based deep eutectic solvents mixtures

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Deep eutectic solvents (DESs) are environmentally friendly solvents formed by combining a hydrogen bond donor and acceptor, resulting in a mixture with a lower melting point than the individual components[1]. While there is extensive research on the electrochemical synthesis of platinum nanoparticles in DES, studies on the chemical reactivity of platinum (II) salts are lacking. This study investigates the reaction of K_2PtCl_4 with the model chelating diamine ethylenediamine (en), using two hydrophilic DESs: choline chloride: glycerol 1:2 (glyceline, GL) and choline chloride: ethylene glycol 1:2 (ethaline, EG). The experiments, conducted in a 70% DES and 30% 1:1 H_2O/D_2O mixture for NMR analysis, revealed that en quickly formed $[PtCl_2(en)]$, which further reacted to produce $[Pt(en)_2]Cl_2$. Reaction products were characterised by 1D (^1H and $^{195}Pt\{^1H\}$) and 2D ($[^1H,^{13}C]$-HSQC and $[^1H,^{15}N]$-HSQC) experiments. Notably, discolouration and precipitation of the purple Magnus salt[2] $[Pt(en)_2][PtCl_4]$ occurred over time. The main difference between the two solvent mixtures was the noticeably slower reactivity in glyceline, due to the much higher viscosity of the solution[3,4]. Diffusion-ordered spectroscopy (DOSY) indicated a lower water molecules mobility in DES mixtures than in H_2O[5], and that reaction products were closely associated with DES molecules. This research opens new perspectives concerning the management of the reactivity of Pt complexes, particularly in their application as anti-cancer drugs, and suggests further investigation in multiple DES types.

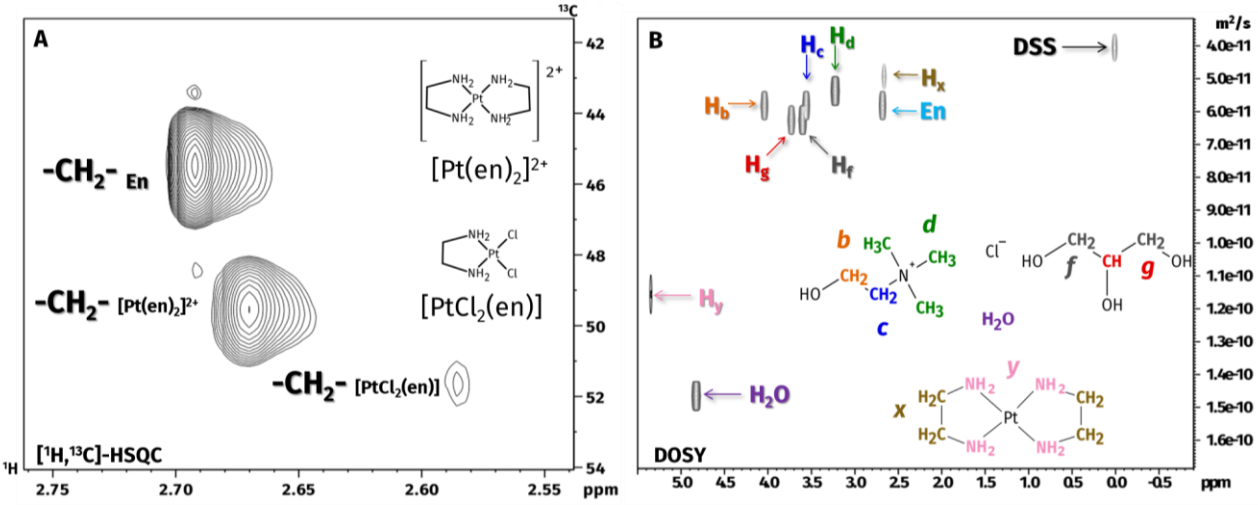

Figure 1: $[^1H,^{13}C]$-HSQC spectrum of en, $[PtCl_2(en)]$, $[Pt(en)_2]Cl_2$ in EG (A) and ^1H DOSY spectrum of GL, en and $[PtCl_2(en)]$ (B)

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Keywords: *Platinum complexes, Green Deep Eutectic Solvents, Multinuclear NMR spectroscopy, DOSY*

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Silk Fibroin as a bioinspired organocatalyst for Michael addition reactions

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Silk fibroin (SF), an attractive natural fibrous protein extracted from *Bombyx mori* silkworm cocoons, has emerged as a highly promising biomaterial owing to its accessibility, physical-chemical properties, and adaptability.[1] Besides the traditional use in textile industry, SF is recognized as a versatile material that has been investigated as an encouraging resource in biomedicine, optoelectronics and many other technological applications.[2] SF has been also successfully used as support for a variety of metal-based catalysts, due to its chemical stability, high temperature resistance and highly hydrophilic structure.[3,4]

In this study we disclose the catalytic activity of SF in the Michael addition reactions of nitromethane to α,β -unsaturated carbonyl compounds. This reaction is one of the main methods for the formation of C-C bonds providing β-nitro-carbonyls adducts suitable for many applications such as the synthesis of pharmaceutical products. [5] The SF catalyst has demonstrated to promote selectively the 1,4 addition of nitromethane to α,β-unsaturated carbonyl compounds under mild conditions, obtaining a library of adducts in almost quantitative yields and with complete diastereoselectivity. Moreover, we illustrate the remarkable recyclability of this catalyst and finally we propose a plausible mechanism based on the probable active reaction sites of SF, provided by molecular dynamics modelling.

Keywords: *Biopolymer, Silk Fibroin, organocatalyst*

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PLA@Croconaine matrix as a photothermal layer: photophysical and thermal investigations

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Polylactic acid or polylactide (PLA) is a readily available, biobased polyester that can be obtained from bio-refinery (from agro-industrial waste). It's an excellent polymer for 3D printing applications, characterized by interesting properties, such as transparency, mechanical strength, biocompatibility, biodegradability, and compostability. These features are the reason why PLA has attracted high interest in lots of applications such as biomedical, food packaging, automotive, electronics, and so forth[1]. Thermal properties of PLA have been widely investigated in the last decades [2,3]. A lot of recently scientific reviews and papers have reported detailed thermal studies of pure PLA or PLA-based composite materials. The chemico-physical properties of PLA can be finely tuned by combining it with proper additives in new composite materials. In the present work, we present our recent results aimed to investigate the properties of a new composite material based on PLA and a functional organic molecule (a croconaine derivatives labelled as CR-BI[4]). We selected a benzo-indolenine based croconaine CR-BI to combine with PLA in a new matrix to manufacture a CR-BI/PLA photothermal layer. Three layers were prepared by dissolving different concentrations of CR-BI (0.1%wt, 0.5%wt and 1%wt) in a chloroform solution of PLA (20 mg/ml), then casting the resulting solutions onto a proper support. The CR-BI show a good affinity with the PLA allowing to realize solid layers with a homogeneous distribution of CR-BI in the PLA matrix. The solid layers of CR-BI/PLA were submitted to investigation in order to determine how the CR-BI component affect photophysical and thermal properties of PLA.

Acknowledgements: This work was financially supported by MUR, project PON ARS01_00869 PERCIVAL- Programma di ricerca n. 03.231- CUP: B95F21001900005, titled "PERCIVAL-Processi di EstRazione di bioprodotti da sCartiagroIndustriali e VALorizzazione in cascata".

Keywords: PLA, Croconaina, Biopolymers, Thermal Study

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Natural urease inhibitors from lignocellulose

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Urea is the main source of N in worldwide crop production, but its rapid hydrolysis catalysed by soil urease resulted in a substantial decrease in fertilisation efficiency. Also, the rising pH impacts plant germination or early growth. Overall, the main problem remains ammonia volatilization, considering the compound itself and contributing to atmospheric pollution by reacting with acid pollutants (e.g., SO_2, NO_x)[1]. Using urease inhibitors as N-stabilizers has been implemented to counterbalance these negative aspects. One of the most used for agronomic purposes is N-(n-butyl) thiophosphoric triamide (NBPT), often co-formulated with urea for a controlled release of both the fertilizer and the urease inhibitor. Catechol and catechol-like molecules have been widely studied as alternatives but many of these compounds have safety issues[1].

In the present work, different aromatic molecules obtainable from lignocelluloses were investigated to understand any possible structure-activity regarding urease inhibition and find sustainable and safe substitutes for commercial urease inhibitors.

The inhibition experiments were performed on Jack bean urease as well as urease naturally present in soil samples. Preliminary results indicate that the phenolic compounds here tested have a wide range of inhibition activity (from 2 to 48%) but no one of them reach the performance of catechol. The best inhibition results were obtained with a bio-oil obtained by pyrolysis of wood at 650°C and 2,6-dimethoxyphenol (Figure 1).

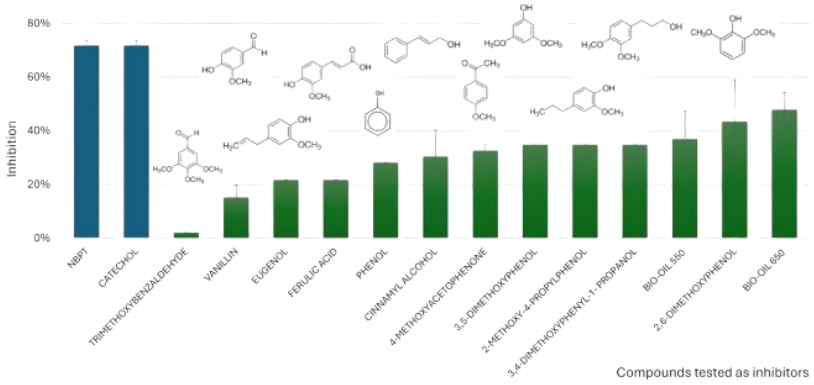

Figure 1. Inhibition of the activity of soil urease achieved by various aromatic compounds, in comparison to NBPT and catechol.

Keyword: *urea, soils, ammonia, environment.*

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An initial assessment of Deep Eutectic Solvents on bacterial photosynthesis

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Deep eutectic solvents (DES) are innovative sustainable solvents characterized by melting points much lower than those of individual components[1]. The decrease in the melting point of the mixture is due to a strong interaction between the components, leading to a less ordered structure that maintains them liquid at room temperature and sustains chemical stability of molecules that are solved into. Most DES are not toxic, generally low-cost, and their preparation is easy and straightforward. Thus, little or no waste is generated in chemical synthesis and no purification is required.

DESs have been shown to maintain the catalytic activity of the membrane photosynthetic enzyme – known as reaction center (RC) – obtained from the purple non sulphur bacterium *Rhodobacter sphaeroides*. Nine different DESs were tested and all but one showed full compatibility with the membrane protein[2].

In this study, we widened our investigation to evaluate the compatibility of DESs toward photosynthetic membrane vesicles cointaining RC and light-harvesting complexes called chromatophores, isolated from the mutant strain R26 of R. *sphaeroides*. Three different DESs were studied, namely TBAB:Gly (1:3), ChCl:EG (1:3) and ChCl:U (1:2) and their effect on the integrity of vesicles was analysed by UV-Vis-NIR spectroscopy.

Acknowledgment: Corso di dottorato di Interesse Nazionale in Processi e Tecnologie Fotoindotti, Ciclo XL, a.a. 2024-2025

Keywords: DES, soluble protein, membrane protein, photosyntetic system

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Chemical Interaction of Monoethanolamine (MEA) with Cooked Soil: A Step Towards the Reformulation of Home Care Products

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Reducing the environmental impact and carbon footprint of commercial cleaning products is a critical challenge for the formulation industry. The ultimate goal of this study is the decarbonization of home care products, specifically spray degreasers, through the exploration of sustainable alternatives to monoethanolamine (MEA). MEA is a widely used component in degreasers and is often included in hard-surface cleaner formulations under the assumption that it act as anti-corrosive agent. Despite that, their direct role in cleaning performance remains poorly understood. This study reveals that MEA's primary function lies in its direct contribution to cleaning performance, particularly through soil softening and dewetting mechanisms.

The cleaning performance of formulations with and without MEA was tested on standard polymerized grease baked on stainless steel plates (IKW soil). The results demonstrate that cleaning performance is primarily dependent on the presence of MEA. To confirm that the degreasing power of dilute MEA aqueous solutions is driven by dewetting in combination with chemical softening of the baked dirt, the possibility of chemical reactions involving MEA was examined. Chemical interactions between MEA and polymerized baked grease were thoroughly studied using FTIR, NMR, and TGA. Sample preparation was carried out to closely mimic the typical conditions of industrial performance tests. Spectroscopic analysis showed that exposing baked soil to MEA solutions modifies the functional groups present in the dirt.

The findings from these analyses were benchmarked against standard industrial performance tests, such as the IKW test, to establish a robust and predictive framework for evaluating alternative molecules to MEA.

From lignocellulosic biomasses to advanced biopolymers in just one step

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Developing economically sustainable processes for lignin valorization remains a significant challenge. Recently, a new paradigm known as "lignin-first" has emerged, focusing on lignin fractionation through biopolymer solvolysis followed by reductive stabilization to prevent biopolymer condensation. [1] Our research centres on ethanosolv processes aimed at achieving high retention of β-O-4 linkages in lignin fractions, using endocarps as feedstocks. Particularly, pistachio dried shells have shown promising results.[2] By optimizing biomass pre-treatment and utilizing microwave-assisted extraction, we achieved a delignification yield exceeding 70%, with lignin fractions primarily composed of S units and retaining approximately 70% β-O-4 linkages. However, the process duration, requiring 10 hours at 80°C, is a drawback. To enhance economic sustainability, we explored a single-step process that simultaneously extracts and functionalizes lignin. This approach eliminates the need for post-processing and enables lignin functionalization with gallic acid[3], thus streamlining the process and reducing costs. The extraction-functionalization process exploits the acid environment of the extraction mixture to perform a microwave-assisted transesterification reaction between the carboxylic acid groups present on the additive molecular structure and the hydroxylic groups presents on lignin structure (Figure 1). Our findings demonstrate that using pistachio shells as feedstock in an optimized ethanosolv process can yield high-quality lignin fractions with significant retention of β-O-4 linkages. While the process duration remains a challenge, the development of a single-step extraction and functionalization method offers a promising path toward more economically viable lignin valorization, transforming lignin from a waste to a versatile material. This integrated approach not only simplifies the process but also adds value to lignin by enabling its functionalization for various applications, potentially leading to broader industrial adoption and enhanced sustainability in biomass utilization.

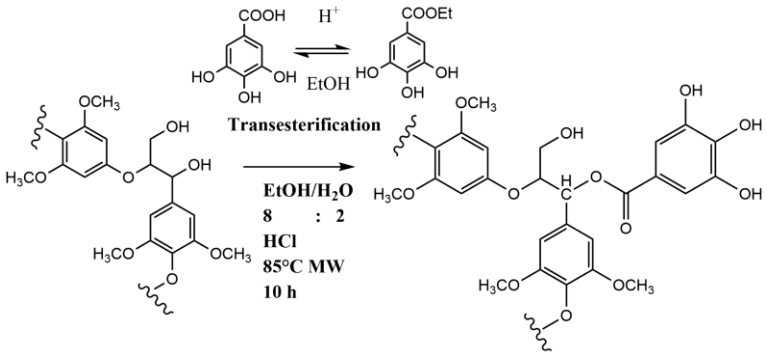

Figure 1: Gallic acid functionalization mechanism trough acid catalyzed transesterification

Keywords: lignin-first, ball miller, microwave-assisted extraction, one-pot functionalization

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Decoding Organic Binders in Art: Hydrogel Micro-Extraction and MALDI-MS for Non-Invasive Identification of Natural Gums

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Natural gums have played a pivotal role in historical painting techniques, serving as binders for the dispersion of pigments on various substrates, including wood panels, canvas, and parchments. These binders often consist of a complex mixture of polysaccharides, proteins, and lipids, which collectively define the artwork's material properties. Understanding their composition is essential for devising effective conservation strategies and restoration treatments. Advances in mass spectrometry (MS), coupled with soft ionization sources like matrix-assisted laser desorption/ionization (MALDI) and electrospray ionization (ESI), allow for molecular profiling and identification of these organic binders[1].

However, when dealing with the diagnostic of artworks, the non-invasiveness is highly preferred, and sampling is discouraged. For this reason, in this study, we developed a rapid and minimally invasive protocol using high-retention hydrogels for *in-situ* sampling and analysis of Arabic, tragacanth, and cherry gums. These hydrogels function as highly effective micro-extractors when applied to artwork surfaces. By incorporating specific enzymes, they enable *in-situ* digestion and capture of oligosaccharides for subsequent MS analysis. Building on earlier methods, where hydrogels loaded with proteolytic enzymes successfully identified protein-based binders such as egg, milk, and collagen[2,3], our approach was tailored to analyze polysaccharides in gum binders. This was achieved by using hydrogels containing exo-1,3-β-galactanase or endo-1,4-β-mannanase. The resulting oligosaccharides were then analyzed and identified through MALDI-ToF-MS, providing detailed insights into the composition of natural gums.

Initial digestion trials were conducted using solutions of Arabic, tragacanth, and cherry gums. To further refine the proposed approach, model samples were created by applying mixtures of these gums and pigments onto parchment. These models facilitated the optimization process, proving the method's effectiveness in handling complex matrices and highlighting its potential for application to heritage materials.

Acknowledgements: This work was supported by Progetto di Ricerca di Interesse Nazionale-PRIN 2022CNNRWZ- REActive GEl for orgaNic bindERs recognition in Artworks (REAGENERA), financed by the Italian Ministero per l'Istruzione, l'Università e la Ricerca (MIUR).

Keywords: *Organic binders, hydrogel, mass spectrometry, non-invasiveness*

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Photonic Nanostructures from organic fluorophores and biosilica

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Diatoms, among the most compelling living organisms for generating nanostructured components, represent a prolific and diverse class of single-celled photosynthetic microalgae. Their mesoporous biomineralized silica shells, known as frustules, encapsulate the organic protoplasm and exhibit remarkable properties, including high surface area, mechanical resistance, distinctive optical characteristics, and mesoporosity[1]. These attributes make frustules highly suitable for various advanced applications in photonics, sensing, optoelectronics, and biomedicine[2]. The remarkable potential of diatoms in nanotechnology is largely attributed to the porous structure and the presence of hydroxyl groups on the surface of their biosilica shells, which facilitate various chemical modifications for targeted applications. These modifications include adsorption of functional molecules and covalent bonding onto the porous frustule surface after isolation from the protoplasm; metabolic incorporation of molecules into the frustule's nanostructure during cell growth; chemical transformation of diatom biosilica into materials that retain the replicated structure but have entirely different chemical compositions. The ability to chemically and biologically modify the composition of frustules offers a versatile approach for engineering nanostructured materials with properties tailored to specific applications[3]. In particular, our study points out that the functionalization of diatoms biosilica with tailored photoactive molecules can represent a powerful tool in order to obtain luminescent micro- and nanostructured biomaterials for applications in biomedicine, optics and photonics.

Acknowledgements: This work has received funding from the European Union Next-Generation EU (PIANO NAZIONALE DI RIPRESA E RESILIENZA (PNRR)–MISSIONE 4 COMPONENTE 2, INVESTIMENTO 3.3–D.M. 117/2023).

Keywords: Diatoms, biosilica, organic fluorophores, nanostructured materials

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Development of P2X7 receptor antagonists for modulating immune response in neurodegenerative disorder with improved drug-like properties

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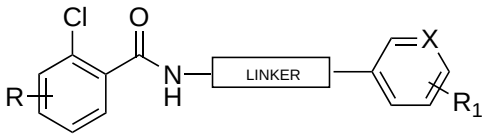
The purinergic P2X7 receptor (P2X7R) is a non-selective cation channel activated by high concentrations of extracellular adenosine triphosphate (ATP). P2X7 is key player in ATP-mediated cell death, inflammation, and immune responses. Owing to its the importance in regulating inflammatory cytokines and the localization on microglia, P2X7R has been the object of intense research efforts as a promising therapeutic target for modulating immune responses in Central Nervous System (CNS) disorders, characterized by chronic neuroinflammation. [1] While significant progress has been made in the identification of human selective P2X7R antagonists, there remained an insufficient number of CNS-permeable antagonist tools that can be to probe in vivo CNS pharmacology.

Starting from a literature survey, we identified three different chemotypes capable of interacting with P2X7R and characterized them in terms of physicochemical properties critical for blood-brain barrier permeability and bioavailability.[2] Next, we selected the most "flexible" molecular scaffold (*Figure 1*). and performed structural modifications to improve the pharmacodynamic and pharmacokinetic profile of the newly designed P2X7R antagonists. The structural modifications were guided by molecular docking studies, leveraging available 3D structures of P2X7R in the Protein Data Bank to preserve crucial receptor-ligand interactions.



R=OCH_3, OCH_2CH_2F
R_1=F, OCH_3
X= N, CH

Figure 1. General structure

We here report on the design, synthesis and biological characterization of a series of 2-chlorobenzamide-based P2X7R antagonists. Their potential application as PET radioligands for in vivo imaging of P2X7R will be also illustrated.

Keywords: *P2X7, antagonist, PET, Central Nervous System*

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Poster Presentations

Bottom-up proteomics for identifying and quantifying soybeans and mustard allergens in processed food matrices

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Food allergy is a significant global health concern, as recognized by the World Health Organization (WHO). Currently, there is no cure for food allergies in sensitized individuals other than the complete avoidance of allergenic ingredients. To address this challenge, European Regulation No. 1169/2011 has established a list of 14 major allergenic foods, including soybean and mustard[1]. Soy and mustard plants are often utilized during wheat cultivation due to their beneficial properties, such as soil nitrogen enrichment, protection against water and wind erosion, enhanced soil biodiversity, and suppression of weed growth. However, these agricultural practices may lead to in-situ cross-contamination of wheat with soy and mustard allergens. Consequently, there is a growing need for analytical methods capable of identifying and quantifying these hidden allergens in complex and processed food matrices[2,3].

To meet the demand for reliable multi-allergen detection, this study aimed to identify and quantify trace amounts of soy and mustard allergenic proteins in naturally contaminated wheat flour and in cookies prepared with the same flour by mass spectrometry (MS) techniques. A bottom-up proteomic approach was employed, leveraging efficient and time-saving protein extraction protocols that used environmentally friendly solvent mixtures. The extracted proteins were enzymatically digested and analyzed using reversed-phase liquid chromatography coupled with low-resolution/accuracy MS. Targeted acquisition was performed using the multiple reaction monitoring (MRM) method[3], focusing on quantifier and qualifier marker peptides for two key allergenic proteins: Glycinin G1 (soy) and 11S Globulin (mustard). The method was validated by evaluating linearity, limits of detection (LOD) and quantification (LOQ), matrix and processing effects using selected marker peptides. Finally, the validated method was applied to quantify soy and mustard allergens in samples, such as flour and incurred cookies, demonstrating its applicability and reliability for allergen detection in processed food products.

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Keywords: *bottom-up proteomics, allergens, mass spectrometry*

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Electrochemical Impedance Spectroscopy Investigations on MnO_2-based Gas Diffusion Electrodes for Zinc-air batteries

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One of the main European objectives regarding electrochemical energy storage is to replace Critical Raw Materials (such as lithium and cobalt) with earth-abundant ones, with the aim of combining high-performance devices with a greener circular economy.

Zinc-Air Batteries (ZABs) represent a viable alternative to conventional lithium-based batteries, for their higher theoretical energy density, environmental-friendliness, safety and affordability [1].

Nevertheless, sluggish kinetics of oxygen electro-catalytical reactions during discharge (Oxygen Reduction Reaction, ORR) and during charge (Oxygen Evolution Reaction, OER) are the main drawbacks with ZABs, resulting in high overpotentials and low efficiency. These issues are accentuated during battery cyclability and worsen over time, leading to degradation of the electrode and of full device [2].

In this scenario, Electrochemical Impedance Spectroscopy (EIS) represents a valid instrument to study the charge transfer ability of materials and to monitor their degradation during operation.

In our work, we synthesized different MnO_2 micro/nanocrystals by hydrothermal synthesis, varying precursors and additives (such as CTAB and ionic liquids, e.g. BMIM-BF_4), and implemented these materials in bifunctional Gas Diffusion Electrodes of Zn air batteries.

We performed EIS at various current densities (from 1 mA/cm^2 to 20 mA/cm^2) to evaluate solid-electrolyte interface and charge transfer resistances occurring during ORR and OER [3]. Furthermore, we monitored the behaviour of our devices during long-term cycling at 5 mA/cm^2 in order to evaluate their stability.

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Keywords: *Zinc-air batteries, nanostructured manganese dioxide, Electrochemical Impedance Spectroscopy*

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Daunian ceramics under the lens: a multi-technique investigation to uncover the past

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This study focuses on the ceramic production of Daunia prior to Greek colonization. Daunian pottery, a hallmark of Apulia, evolved through distinct phases, from the Protogeometric to the Subgeometric periods, reflecting advancements in both style and technology. The primary goal is to investigate the raw materials and manufacturing methods employed by the Daunian people before Greek influence. Polychrome tempera vases from the 10th–9th to the 4th century BCE, collected from two Daunian sites, Cannae della Battaglia and Ordona, were examined using non-invasive or minimally invasive techniques, including LA-ICPMS, Raman spectroscopy, and SEM.

The findings indicate differences in the raw materials used for pottery production between the two sites, while each site maintained consistent raw material selection and production methods throughout the studied period (10th–9th to 4th century BCE). Additionally, it was determined that the surfaces of the pottery were coated with a mixture of clay and bone ash prior to decoration. This preparation enhanced the brightness of the vase surface and accentuated the decorative colors.

Regarding the red, black, and brown decorations, the study suggests that *terre rosse* (a common sedimentary material in Apulia) was utilized. Black decorations likely incorporated manganese oxides/hydroxides and charcoal, while brown tones were achieved using manganese oxides/hydroxides. The analysis of mineral composition provided crucial insights into the manufacturing process, particularly the firing temperature and duration.

The study aids in uncovering the raw materials and production techniques used by the Daunian people during the pre-Greek colonization era.

Keywords: *Archaeometry, Pottery, Pigments, Daunia*

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Self-powered wearable biosensor with stencil-printed carbon nanotube electrodes for monitoring sweat ethanol levels

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In recent years, wearable electrochemical biosensors have gained significant attention due to their potential for affordable, real-time health monitoring, providing a solution to the limitations of traditional, bulky, and expensive medical equipment [1]. These devices are designed to continuously and remotely monitor health metrics, offering valuable data without the need for specialized equipment or clinical visits. A major challenge in this field is the development of self-powered biosensors, which eliminate the need for external batteries or power sources [2]. Instead, these devices generate the necessary energy through enzymatic reactions or biorecognition components, making them particularly suitable for applications such as alcohol abuse detection, where traditional methods are costly, time-consuming, and impractical for continuous monitoring [3].

This work introduces a novel self-powered wearable biosensor for alcohol detection in sweat. The biosensor is based on water-based graphite ink modified with multiwalled carbon nanotubes (MWCNTs), offering a biocompatible, scalable, and environmentally friendly solution for electrode fabrication. Unlike traditional inks that use organic solvents, the water-based ink improves conductivity and enhances the stability of biological components. The device employs an innovative two-electrode system, where electrodeposited catalysts and immobilized enzymes enable self-powered alcohol detection. The biosensor demonstrated a linear detection range from 0.01 to 0.3 mM, with a detection limit (LOD) of 3 ± 1 µM, a sensitivity of 64 ± 2 $\mu W \cdot mM^{-1}$, and a correlation coefficient of 0.98 (RSD 8.1%, n = 10 electrode pairs). It exhibited robust operational stability (over 2800 s with continuous ethanol turnover) and excellent storage stability (approximately 93% of the initial signal retained after 90 days). Finally, the biosensor array was integrated into a wristband and successfully evaluated for continuous alcohol abuse monitoring. This proposed system demonstrates promising attributes for use as a flexible, wearable biosensor employing biocompatible water-based inks, with potential applications in forensic contexts.

Keywords: *Wearable biosensor, Water based conductive inks, Ethanol biosensors, Enzymatic biofuel cells*

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Choline acetate as a novel ionic liquid for Sonogashira cross-coupling reaction

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Sonogashira reaction is the main synthetic tool suitable to perform the cross-coupling of terminal alkynes with aryl or vinyl halides, assembling Csp-Csp² bonds an affording highly unsaturated skeletons such as arylacetilenes or enynes, that are the subunits of many bioactive compounds, drugs and natural products[1]. The classical Sonogashira coupling needs for toxic organic solvents, stoichometric quantities of bases and noble metals or other critical materials such as copper. In line with Green Chemistry principles, many efforts in today's research are devoted to the development of new catalytic systems to lead the Sonogashira reaction under sustainable conditions. In this context, heterogeneous catalytic systems[2], metal-free conditions[3], phosphine-free protocols[4] and microwave irradiations[5] have been proposed until now.

Much less investigated, in this field, is the use of ionic liquids (ILs), the non-volatile, non-flammable, organic salts which are liquid at room temperature, that are considered the environmentally friendly alternative to common toxic organic solvents (e.g. halogenated hydrocarbons, alcohols, acetonitrile, DMF etc.).

In this communication, an unprecedented copper-free Sonogashira protocol carried out in Choline Acetate is presented. Choline ((2-Hydroxyethyl) trimethylammonium) is the well-known subunit of natural compounds that gives rise to a class of green and non-toxic ILs. Choline acetate belongs to the class of basic ILs due to the basicity of the anion acetate. It presents a set of advantages if compared to the classical tetraalkylamonium and imidazolium ILs such as lower thermal degradation and lower solubility problems during the work-up. The coupling protocol in this medium appears to be innovative and convenient due to the mild and green conditions.

Keywords: *Cross-coupling, Sonogashira, Choline acetate*

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Identification of X-ray irradiated peanuts by DNA comet assay and HS-SPME/GC-MS analysis

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Peanut is one of the most widely used legumes due to its nutrition and taste. During the storage, this product is susceptible to pest infestations and microbial contamination. X-ray Ionizing radiation is a non-thermal, safe and effective technology used to inactivate pathogens and may positively affect peanut preservation [1]. The European regulatory framework included the legumes matrices into the list of food and food ingredients which may be treated with ionizing radiation [2] up to 1.0 kGy, therefore control methods to identify any illicit treatments are essential for Member States. The UNI EN 13784:2002 DNA comet test is a rapid and sustainable screening tool for analyzing irradiated vegetables in terms of DNA breaks due to X-rays. However, thermal, mechanical and irradiation DNA damage can be similar, therefore a confirmatory method is mandatory. HS-SPME/GC-MS is a green alternative to standard method UNI EN 1785:2003 for the qualitative determination of 2-dodecylcyclobutanone (2-DCB) known as radiation marker [3]. 2-DCB is specific compounds generated from triglycerides containing palmitic acid by irradiation of fat-rich foods. In this work, shelled raw peanuts were irradiated in plastic bags using a low-energy X-ray irradiator at dose levels of 0.5, 1.0 and 1.5 kGy. The comet DNA was appropriately validated using 1.0 g of crushed peanuts and optimized sedimentation and lysis times to 45 minutes for both. The HS-SPME/GC-MS analysis, performed using headspace extraction with PDMS fibre and SIM mode acquisition, was carried out on 5.0 g of ground samples in a 20 mL glass headspace vial containing 5 ml of deionized water. The identification criteria of 2-DCB were compliant with EN ISO 1785:2003. In not treated peanuts, used as control, intact cells without comets were observed while the irradiated samples showed comets with a homogeneous pattern and the fluorescence intensity is proportional to the treatment dose. The screening results were confirmed by the presence of 2-DCB only in the irradiated samples. Moreover, interference was not highlighted and the area of 2-DCB was increased directly to dose treatment, confirming the selectivity and linearity of HS-SPME/GC-MS method for the selected matrix. The outcomes confirmed the possibility to use the UNI EN 13784:2002 DNA comet assay together with HS-SPME-GC/MS for vegetables products analysis within official laboratories for routinely control activity.

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Keywords: *DNA comet assay, Food Irradiation, HS-SPME/GC-MS, Peanuts*

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Preliminary study for the development of new dual agonists of PPAR and FXR for the treatment of Metabolic Dysfunction-Associated Steatohepatitis (MASH)

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Metabolic Dysfunction-Associated Steatotic Liver Disease (MASLD) has emerged as a major hepatic disorder characterized by excessive fat accumulation in the liver[1]. This condition, often associated with metabolic syndrome, can progress to more severe forms such as steatohepatitis (MASH), fibrosis, cirrhosis, and hepatocellular carcinoma[2]. Currently, lifestyle modifications and weight loss remain the primary treatment options for MASH[3]. However, the multifactorial nature of the disease necessitates the development of novel therapeutic approaches. A multi-target approach which offers a promising strategy is considered the concomitant activation of the Farnesoid X Receptor (FXR) and Peroxisome Proliferator-Activated Receptors (PPARs)[4]. Over the last twenty years, our research group has extensively focused on the therapeutic potential of PPAR agonists. Building upon previous findings, we have now identified some compounds that, besides exhibiting potent agonist activity toward both PPARα and PPARγ receptors[5], possess also antagonist activity towards FXR. One of these molecules (RT206) (Fig.1) is currently under investigation representing a suitable scaffold to be modified in the attempt to achieve new compounds endowed with agonistic activity towards both types of nuclear receptors and to evaluate its potential efficacy in a MASH experimental model.

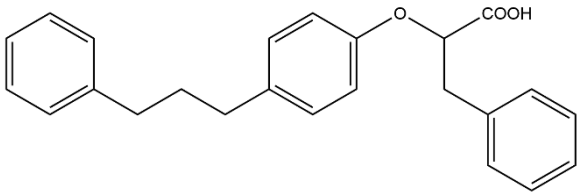

Figure 2: Structure of RT206

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Keywords: *FXR, PPARs, MASH, Multi-Target*

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Edible Amperometric Biosensors for Intestinal Monitoring of Glucose Levels

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As per the World Health Organization, approximately 422 million individuals, around 5% of the global population, have diabetes, making it a significant health concern.[1,2] Predicted to become the seventh leading cause of death, diabetes is a serious threat due to its associated complications, including cardiovascular disease, blindness, amputation risk, and kidney failure. Managing blood glucose levels is crucial for delaying these complications, but it's a challenge due to significant variability, especially in severe cases. This need for precise monitoring has led to a thriving market for glucose biosensors valued at over 15 billion EUR annually. However, challenges persist, primarily in scaling up biosensor production with multiple costly biological elements. To address this challenge, the scientific community is working on developing reusable biosensing platforms with long-term stability.[3]

Although implantable and minimally invasive sensors offer the advantage of continuous monitoring, their chemical compositions pose significant regulatory challenges for routine usage. As a result, there is a growing emphasis on developing diagnostic devices that are biodegradable, bioresorbable, or ingestible to overcome this limitation. In this regard, we have addressed the very important challenge of tailoring and designing novel conductive smart carbon-based inks completely biocompatible and edible to develop biocatalytic biosensors able to monitor the intestinal absorption of glucose in type 2 diabetic (T2D) patients. We employed a Design of Experiments (DoE) approach like Face Centered Design to optimize processing variables and enhance ink performance, providing a unique model for formulating edible carbon-based inks.[4]

Keywords: *Glucose monitoring, biocatalytic biosensors, edible inks, design of exepriments.*

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Functionalized MALDI matrices for the analysis of low molecular weight compounds

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The application of matrix-assisted laser desorption/ionization mass spectrometry (MALDI MS) to low molecular weight compounds analysis has stayed challenging due to the spectral interferences of ionizable conventional organic matrices in the low *m/z* range. To overcome this issue, alternative methodologies based on rationally designed organic matrices have been proposed [1].

The purpose of this investigation was to synthesize novel functionalized MALDI matrices able to react with small amines and alcohols with the aim of analyzing these low-mass compounds avoiding interfering matrix background. The functionalization was carried out by nucleophilic substitution of two different p-hydroxy compounds, 4-hydroxybenzoic acid (4-HBA) and alpha-cyano-4-hydroxycinnamic acid (CHCA), with a 2,4,6-trichloro-1,3,5-triazine (TCT) in the presence of a base [2]. Trichloro-triazine, also known as cyanuric chloride, has reported a marked reactivity toward hydroxyl and amine groups [3]. In our experiments, we first carried out the reaction between CHCA or HBA and TCT exploiting the presence of -OH residue on the matrix; the resulting product was characterized by ATR-IR and NMR spectroscopies and MS analysis. Thus, the other two chlorines on TCT-CHCA or TCT-HBA can further react with amines or alcohols allowing to increase the molecular weight of these small compounds towards higher *m/z* ratio. It becomes an in-situ derivatization aimed also to improve the sensitivity of the investigated compounds.

The reactive TCT-CHCA or TCT-HBA matrices were tested with different amino acids, such as phenylalanine, glycine, isoleucine and cysteine. Preliminary results are reported in this communication.

Keywords: *MALDI-ToF, Matrix, Triazine, Amino acids*

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Volatolomics based on HS-SPME/GC-MS and multivariate analysis for the characterization of volatiles in peels of prickly pear and pomegranate

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Over the last twenty years, the interest in reusing plant-based by-products has increased significantly worldwide, with a view to encouraging the transition towards a circular economy. Therefore, by-products of fruit and vegetable industry represent an important resource to be reused, as an example by their addition to foods with the aim of increasing their content in nutraceutical substances[1,2]. However, the addition of these by-products could lead not only to changes in both the sensorial and acceptability of the food product, but also in the composition of volatile compounds. Therefore, it is fundamental to characterize the volatile profile of the processed by-products before using them as nutraceutical food additives, in order to guarantee to the final consumer the sensorial acceptability of the enriched food product[3].

In this study, the profile of the volatile components (VCs) of fresh and dehydrated prickly pear and pomegranate peels has been analysed by a volatolomic approach, based on headspace solid phase micro extraction, gas chromatographic separation and mass spectrometry identification (HS-SPME/GC-MS), followed by a multivariate statistical analysis of the results. The use of three SPME fibres with different polarities has allowed a broader extraction of VCs in the different kinds of samples. The use of both a database of spectra and the linear retention indices allowed an accurate identification of the VCs extracted from the by-product samples. Lastly, a proper multivariate statistical analysis of the obtained results has evidenced the differences in the volatile profile of the two types of fresh and dehydrated peels and has allowed the identification of the best parameters of the dehydration process. These results can allow the useful exploitation of these by-products for the development of new foods with a high added value.

Keywords: *volatolomics, agro-food by-products, HS-SPME/GC-MS*

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Advancing sensor technology: real-world applications of MIP-based sensors in Green Analytical Chemistry

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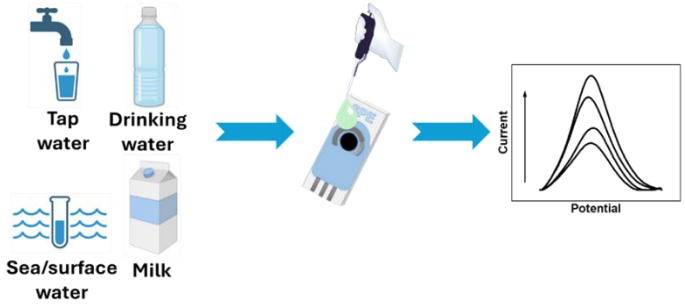
As there is a need for sustainable and environmentally friendly analytical methods, "green analytical chemistry" (GAC), a subfield of contemporary analytical chemistry, is proposed as a way to reduce the use of toxic reagents, limit waste generation, and encourage energy-efficient operations while reducing environmental impact[1]. Chemical sensors based on molecular fingerprint polymers (MIPs) have proven to be tools that meet GAC standards and principles, creating new, more efficient and environmentally friendly ways[2]. MIPs are designed to identify target molecules and function similarly to natural receptors in biological systems. Therefore, they can be used in the future for food safety analysis, medicine, and environmental monitoring due to their high selectivity, sensitivity, and resilience. Advantages of MIP-based sensors include the ability to employ electrochemical methods that allow the use of miniaturized transduction elements (screen-printed electrodes), limiting the need for reagents and solvents, and the potential for regeneration strategies that reduce the overall environmental impact of sensors while facilitating daily monitoring at reduced cost and time. In addition to presenting some recently developed sensors[3–5], optimized for monitoring in complex matrices such as milk, tap water and surface water, this presentation explores the integration of MIP-based sensors developed through GAC principles. Research is moving toward the next generation of sensors that will make monitoring environmental contaminants, early diagnosis in hospitals, and food safety checks easy and reliable on a daily basis..



Schematic representation of environmental monitoring and food analysis.

Keywords: *Green Analytical Chemistry (GAC); MIPs; Electrochemistry; Miniaturized Sensors.*

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Plasma-Based Modification of Tin Halide Perovskite Interfaces for Photovoltaic Applications

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Tin halide perovskites (THP) are one of the most appealing and less toxic alternatives to lead-based perovskite solar cells, which have gained increasing interest in recent decades due to their exceptional optoelectronic properties, straightforward processing and efficiencies comparable to those of silicon solar cells. Despite the outstanding properties of THPs, one of the main disadvantages of this class of materials is the intrinsic tendency of tin (II) to oxidise over time, leading to p-doping of the material and the consequent rapid decay in performance of photovoltaic devices. Engineering the surface passivation of tin perovskites is one of the key strategies to address both stability and performance enhancement of solar cells, for example by using reducing agents, such as hydrazine or some Lewis bases, designing lower dimensional or mixed perovskites, tailoring the composition and/or modulating the crystal orientation.

Among the various approaches investigated, mainly solvent-based, we explored the innovative use of plasma as a solvent-free, reproducible and scalable approach, [1,2] to gently treat the material surface and limit its oxidation. A N_2-fuelled plasma treatment was carried out on a DMSO-free $FASnI_3$ perovskite surface [3], as DMSO is known to oxidise tin itself. A plasma reactor directly located inside the glove box was used and mild power and flux conditions were set. Through chemical, optical and morphological analyses, it was shown that this treatment influenced the ageing of the material by generating transient active species on the perovskite surface, inhibiting the tendency of tin (II) to oxidize, probably due to a modulation of surface defects. As a result, power conversion efficiency (PCE) distribution of stored devices treated for 2 s appears to be slightly higher in value and sharper that that of the reference devices. Therefore, the results of the present work are of great importance because the suppression of the intrinsic tendency of tin (II) to oxidize to tin (IV) was achieved with a non-invasive technique as plasma, which can be easily implemented within large-area production facilities, increasing the potential of alternative lead-free perovskite photovoltaics.

Keywords: *Lead-free Perovskites, Plasma Treatment, Interface Engineering, Solar Cells*

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Tailoring the corrosion behaviour in body fluids of superplastically formed magnesium alloy resorbable implants by means of surface coatings

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Magnesium alloys are potential materials for biodegradable orthopedic implants due to their mechanical characteristics and biocompatibility. However, challenges in manufacturing Mg-based prostheses include selecting and designing suitable and flexible manufacturing processes to create complex shapes (e.g., mimicking the geometry of human bones) and controlling the magnesium degradation rate in body fluids through surface coating methods. Among flexible sheet metal forming processes, superplastic forming (SPF) allows to produce customized and complex-shaped implants characterized by a satisfying shape accuracy and surface quality[1]. SPF can affect the microstructure and, thus, the alloy corrosion resistance, whose value is crucial in influencing the biodegradation rate. In the present contribution, a pulsed laser deposition of hydroxyapatite (HA)[2] coating and a phosphate chemical conversion coating[3] (see Figure 1) were applied to AZ31 Mg alloy components, formed by SPF process, to modulate their degradation rate. Chemical-physical characterizations, electrochemical corrosion tests and electrochemical impedance spectroscopy were performed to assess the beneficial effect of the applied coating on the corrosion behaviour of the superplastically formed AZ31 Mg components.

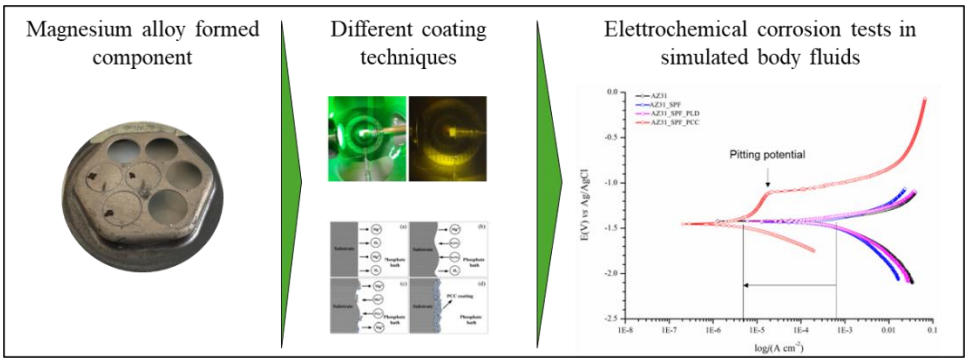

Figure 3 Scheme of the adopted approach

Acknowledgements: The authors would like to acknowledge the funding provided by the Italian Ministry of University and Research (project acronym: CONTACT; code: ARS01_01205).

Keywords: *Electrochemical corrosion tests; Temporary Prostheses; Pulsed Laser Deposition; Phosphate chemical conversion coating; Hydroxyapatite; Magnesium alloy*

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Characterization of atmospheric particulate matter by ATR-FTIR spectroscopy in the framework of TOX-IN-AIR project

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The aim of TOX-IN-AIR project is the evaluation of the role of natural and anthropogenic sources on the toxicological potential of fine atmospheric particulate matter ($PM_{2.5}$). $PM_{2.5}$ is a major risk for public health, potentially leading to millions of premature deaths per year worldwide[1]. The identification of main chemical components linked to toxicity effects of $PM_{2.5}$ samples represents therefore a major challenge for the scientific community. For this purpose, data arising from acellular and cellular toxicity tests are crossed with compositional data obtained by means of different analytical techniques. In this context, attenuated total reflectance Fourier Transform infrared (ATR-FTIR) spectroscopy represents a powerful tool providing prompt and valuable information on the main functional groups present in $PM_{2.5}$ samples. During the measurement campaigns, $PM_{2.5}$ samples have been collected simultaneously on quartz and teflon filters using a dual-channel automatic sampler. Quartz supports were found not appropriate for ATR-FTIR analysis, while PM deposited onto teflon filters was found to produce spectra with satisfying signal to noise ratio. In this contribution we present the optimization of acquisition and processing of $PM_{2.5}$ ATR-FTIR spectra, to collect reliable and accurate information on functional groups possibly involved in toxicity effects that will be correlated with elemental composition obtained by ED-XRF technique.

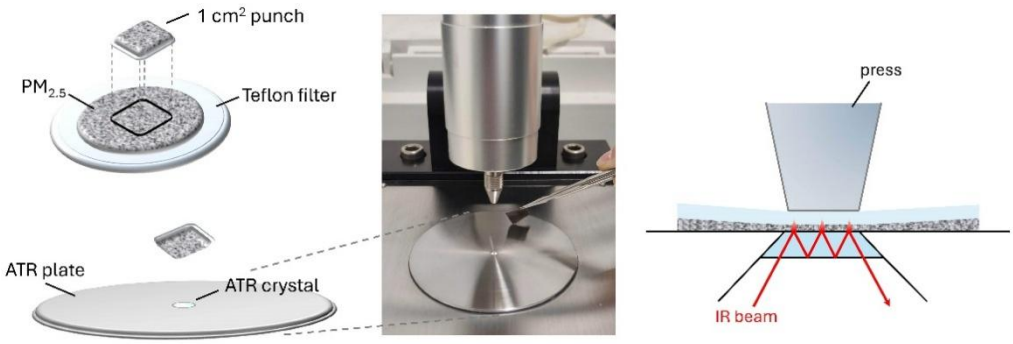

Figure 1: $PM_{2.5}$ sample placement for ATR-FTIR analysis

Acknowledgements: TOX-IN-AIR project is funded by the European Union, NextGenerationEU, Ministero dell'Università e della Ricerca, Call PRIN 2022 PNRR – Project P2022JKP2S, PNRR, Missione 4, Componente C2, Investimento 1.1. CUP B53D23033620001.

Keywords: *atmospheric particulate matter, ATR-FTIR spectroscopy, ED-XRF, teflon filters*

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Sustainable Mechanochemical Approach for Graphene-Based Pellet Production in Additive Manufacturing

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Since its isolation in 2004[1], graphene has garnered significant interest due to its remarkable properties, including high conductivity, mechanical strength, and flexibility, making it a material with immense scientific and industrial potential. Despite its promise, the industrial application of graphene-based materials (GRMs) has been limited by the use of graphene oxide (GO) in most processes. While GO offers easier processing and functionalization, it does not retain the same exceptional electronic properties as pristine graphene. Instead, a major challenge with using pure graphene is its poor solubility, which makes it difficult to manipulate and integrate into materials. This has led to the development of functionalization methods that often compromise the intrinsic properties of graphene, increase processing costs, and lack scalability.

In this work, we present a sustainable, scalable, and solvent-free approach for the non-covalent functionalization of plastic microparticles with pristine graphene. This mechanochemical method involves embedding graphene onto the surface of polymeric particles, preserving its unique properties and minimizing safety risks associated with handling volatile graphene powders. We functionalized Polymethyl methacrylate (PMMA) and polypropylene (PP) with varying amounts of graphene under controlled environmental conditions using a rotary shaker to ensure optimal interaction, while preserving the integrity of both the polymeric particles and the graphene. The resulting materials were characterized using electron microscopy techniques (SEM) and thermogravimetric analysis (TGA), confirming a uniform distribution of graphene and strong particle adhesion.

This process not only produces stable, conductive nanocomposites but also enables their direct use in advanced manufacturing processes, such as microinjection moulding. Our approach bridges material science, advanced manufacturing, and green chemistry, addressing key barriers in graphene industrialization and paving the way for innovative applications in nanocomposite fabrication and device engineering.

Acknowledgements: PRIN 2022 – finanziato dalla Comunità Europea – Next Generation EU - PNRR M4.C2.1.1 MAGELLANO MAnufacturing systems for Graphene nanocompositEs and their appLications as embedded eLectrochemicAl seNsors in Lab-On-chip (grant number: 2022NRMS4X) CUP: B53D23008860006;
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Keywords: graphene, nanocomposites, micro-injection moulding, mechanochemical

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On-demand bioresorbable opto-electronic sensors for in-vivo and in-situ monitoring of chemotherapeutic drugs and biomarkers

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Bioresorbable and biodegradable materials, which dissolve into biocompatible by-products, offer a unique opportunity to create advanced electrical, optical, and sensing components. These components can integrate seamlessly with the human body, enabling direct access to organs, tissues, and biofluids, with significant implications for personalized medicine and wellness applications[1]. Despite progress in developing bioresorbable systems, key challenges remain, including the limited lifetime of components, stability of power sources, controlled material dissolution, in vivo chemical sensing, and long-term biocompatibility [1].

The RESORB project, funded by the EIC PathFinder Open, aims to develop in-vivo bioresorbable sensing systems for chemotherapeutic drug monitoring, such as doxorubicin. These systems will integrate dissolvable electrical and optical devices, power sources, and chemical receptors, enabling real-time drug tracking without secondary device-retrieval surgeries, which can risk tissue damage or infection. As part of the RESORB project, a key goal is to integrate the biodegradable doxorubicin receptor with the bioresorbable transducer to create an effective sensing material. Molecular imprinting (MI) was selected to design an artificial receptor for doxorubicin. This technique forms polymeric matrices with recognition sites tailored to the target molecule. These sites are created during polymerization around a template molecule, which is then removed, leaving cavities matching the target's size, shape, and functional groups[2].

In our approach, porous silica embedded in biodegradable poly(lactic-co-glycolic acid) (PLGA) hydrogels is functionalized with polypyrrole (PPy)-based molecularly imprinted polymers (MIPs). This combination offers structural support, biodegradability, and selective doxorubicin recognition. In vitro studies confirmed the sensor's ability to detect doxorubicin via UV-Vis spectroscopy and fluorescence. Biocompatibility tests in laboratory animals revealed no rejection, behavioral changes, or toxicity, confirming material safety. Future studies will focus on the sensor's complete resorption and real-time in vivo doxorubicin detection

Acknowledgements: This work was funded by the European Union Horizon Europe program under grant agreement No 101046946 (RESORB).

Keywords: bioresorbable sensors, drug monitoring, optical sensors, molecularly imprinted polymers (MIPs)

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Novel molecularly imprinted polymers (MIPs) based on natural phenols combined with Au nanoparticles for sensing applications

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The development of highly selective and sensitive electrochemical sensors is a major goal in modern analytical chemistry. Electrochemical polymerization provides an efficient and sustainable method for modifying sensor surfaces with polymeric receptors. This approach aligns with "green chemistry" principles, minimizing the need for additional reagents and volatile solvents while enabling precise control over polymer features. Compared to traditional chemical synthesis, electro-polymerization is faster, simpler, and produces highly stable films, making it an attractive choice for sensor development [1]. Electropolymerization is a widely used technique for modifying electrochemical transducers with molecularly imprinted polymers (MIPs), which are materials designed to mimic antibodies and exhibit high selectivity and affinity for target molecules. However, the effectiveness of electropolymerization is often limited by the availability of appropriate functional monomers [2].

This study proposes an innovative strategy for MIP fabrication using electropolymerizable natural phenolic antioxidants, such as caffeic acid (CA) and gallic acid (GA), as functional monomers. The approach involves utilizing these polyphenols to modify gold nanoparticles (AuNPs) to use during the polymerization step, integrating them in the resultant polymer matrix. The aim is to obtain MIP-based sensitive materials leveraging AuNPs conductivity and catalytic properties, facilitating the formation of a tailored polymeric structure. The target molecule under investigation in this study is 2-(2,4-dichlorophenoxy) propionic acid (2,4-DP), a member of the chlorophenoxy herbicides group, recognized as one of the priority pollutants on the European list. [3]. Currently, experimental efforts are focused on optimizing the polymerization conditions required for fabricating MIP tailored to 2,4-DP. This involves a detailed exploration of various experimental parameters to maximize both the sensitivity and specificity of the polymer receptor toward the target molecule. Specifically, the experimental workflow encompasses the screening of monomer concentration and monomer/AuNPs ratio, together with the exploration of the synthesis parameters during the cyclic voltammetry, such as scan cycles, scan rate, and potential range.

Preliminary results indicate the successful deposition of polyphenol-based polymers on modified electrodes, with uniform coatings and stability across both aqueous and organic media. This versatile and eco-friendly strategy, leveraging natural materials and low-impact procedures, shows promise for developing advanced electrochemical sensors to enhance environmental monitoring and safeguard ecosystems.

Keywords: *Molecularly imprinted polymer, natural phenols, electrosynthesis, electrochemical sensors.*

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Electrosynthesis of Zinc Oxide-based nanoantimicrobials with Benzalkonium Chloride: Optimization and Analytical characterization

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Zinc oxide (ZnO) is a material of significant interest in different fields, including biomedical, and microelectronics industries, due to its biocompatibility, intrinsic antimicrobial activity, and semiconductor properties. When used in nanostructured form, it exhibits unique chemical-physical properties that allow control and modulation of these characteristics, depending on the intended application.

This work focuses on a ZnO synthesis methodology[1,2,3] that has been developed in our research group by means of chemometric tools. The method is based on a green hybrid electrothermal sol-gel approach, in which the sacrificial zinc electrolysis in sodium hydrogen carbonate solution (30 mM) is combined with typical strategies applied in sol−gel routes to achieve morphological control. Specifically, benzalkonium chloride (BAC) was used as stabilizer. Optimization was carried out to maximize the process yield and to gain a tight control on the morphology of ZnO nanostructures (ZnO-NSs). In a first step, the most influential experimental parameters in the synthesis process were identified and evaluated. Subsequently, a 3-level design of experiments based on the Central Composite Design (CCD) model was defined and applied.

The analytical characterization of the reaction products was performed by combining transmission electron microscopy (TEM) with spectroscopy analyses, including UV-Vis and ATR-FT-IR. The relevant results were used to correlate the chemical composition and morphology of the material with the experimental conditions used during the synthesis. A comprehensive overview of the optimized process will be provided, in view of the final industrial scale-up of the electro-synthesis process.

Acknowledgements: M.I. acknowledges the financial support from the ERC SEEDS UNIBA programme, project H93C23000660001, "REAL - More for less: REthinking AntimicrobiaL materials".

Keywords: Antimicrobial, BAC, Electrosynthesis, Experimental design

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Preliminary ^{1}H-NMR characterization of stabilized grape pomace extracts

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Grape pomace is a natural source of nutraceutical compounds with multiple bioactive molecules[1] that could be exploited also to preserve healthy ageing and preventing chronic age-related diseases improve age-related cardiovascular diseases[2].The aim of our research is to characterize, by ^{1}H-NMR spectroscopy, aqueous grape pomace extracts, identifying the molecules, as polyphenols, with nutraceutical properties. Nuclear Magnetic Resonance Spectroscopy (NMR) is widely used in in food science, and human nutrition[3] since it is a non-invasive, high reproducible and quantitative technique that provides detailed information on molecular structures on specific molecules or complex mixture. A preliminary characterization of grape pomace aqueous extract powder, dehydrated at 90°C for 5 minutes, was carried out. The ^{1}H NMR spectrum, with water signal suppression, was acquired on a Bruker Avance III 600 MHz Ascend NMR Spectrometer.

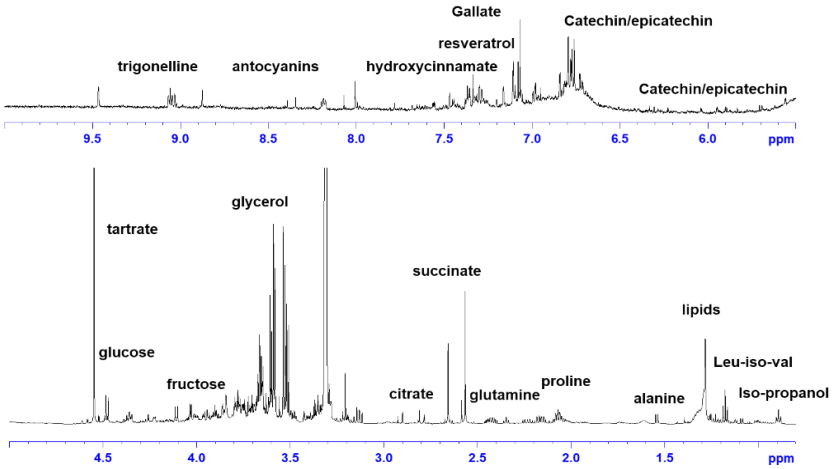

Figure 1: Representative ^{1}H NMR spectrum of GPE. Expanded areas in of (0.5-5 ppm), aliphatic region and (5.5-9.5) aromatic region is reported. The peaks of relevant identified metabolites are labelled.

The resulting spectrum showed a complex pattern of signals due to the presence of different compounds, as sugars, amino acids, organic acids, and polyphenols. The application of this technique could help in the valorisation of stabilized grape-pomace leading to explore possible reuse of grape pomace also obtaining bioactive-compounds added product. Further studies of metabolic alterations induced by digested grape pomace extracts in culture of intestinal epithelial cells and assessment of their stability after enzymatic digestion process are under investigation.

Acknowledgements: The authors thank WINPROAGE project, "WIne by-products metabolomic profiling in Natural chemoPRevention Of vascular AGEings – (: P2022TKYNN); Bando PRIN 2022PNRR- Settore ERC LS 4 "Physiology in Health, Disease and Ageing" financed by the NextGenerationEU plan, Mission 4, Component C2, Investiment 1.1.

Keywords: *grape pomace extracts, polyphenols, ^{1}H NMR spectroscopy*

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Heavy metals and metalloids in blackspotted smooth-hound sharks (*Mustelus punctulatus*) from the Southern Adriatic: contamination and dietary safety

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The bioaccumulation of heavy metals and metalloids in apex marine species raises critical concerns for both ecosystem and human health. In this study, the concentrations of 14 heavy metal(oid)s, in the kidney, liver, brain, and muscle tissues of blackspotted smooth-hound sharks (*Mustelus punctulatus*) collected from the Southern Adriatic Sea were measured. The determinations were performed using three different analytical techniques: ICP-OES, GFAAS, and TDAAAS, after mineralizing the samples with a microwave digestion system. The findings reveal significant patterns of contamination, with males exhibiting notably higher levels of Ag and Hg than females, and accumulation trends indicating the kidney and liver as primary sites for these contaminants. No significant relationship was found between metal(oid) levels and body size, and health metrics, such as the condition factor and hepatosomatic index, suggested that metal(oid) accumulation did not visibly affect shark health in this sample. Of particular concern, As concentrations in all samples exceeded the regulatory maximum level, averaging approximately 7 times the allowable threshold. Hg levels were also elevated, with 57% of muscle tissue samples surpassing EU safe limits. Following US EPA guidelines, for non-carcinogenic risk related to Hg, the maximum allowable number of monthly meals is limited to just 1.1 for adults and 0.5 for children, highlighting significant limitations on safe intake for these groups. Comparisons with *M. mustelus* from the Tyrrhenian Sea [1] show that the Southern Adriatic *M. punctulatus* harbors higher Hg levels, raising greater concerns for consumers in this region.

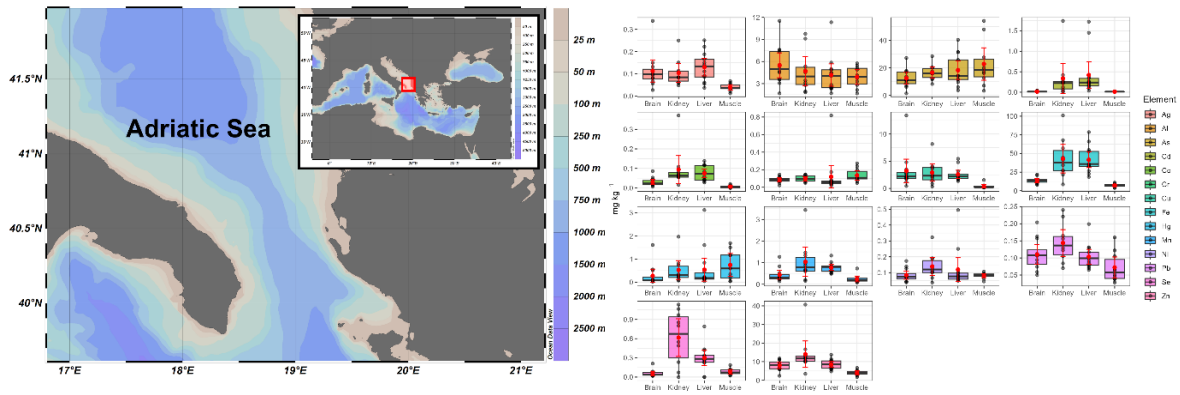

Figure 1: Sampling location and heavy metal(oid) concentrations in M. punctulatus tissues.

Keywords: *mercury, arsenic, conservation, toxicity, pollution, elasmobranch*

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1-Oxa-2,6-diazaspiro[3.3]heptane as a New Potential Piperazine Bioisostere – Flow-Assisted Preparation and Derivatisation by Strain-Release of Azabicyclo[1.1.0]butanes

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The development of novel strained spiro heterocycles (SSHs) as bioisosteres for aromatic or non-strained aliphatic rings is highly sought after, given their potential to impart improved physiochemical properties and improved target selectivity as a consequence of their high molecular rigidity and predictable vectorization. Their high molecular rigidity and predictable vectorization can enhance drug-likeness, target selectivity and clinical success. 1-oxa-2,6-diazaspiro[3.3]heptane (ODASE) is reported as a novel potential SSH-bioisostere. We demonstrate through theoretical studies the potential of this strained spiro heterocycle to act as a bioisostere for piperazine. We have developed its synthesis from the highly strained azabicyclo[1.1.0]butyl intermediate through a robust and mild flow technology two-step protocol. Its stability towards medicinally relevant N-functionalisation protocols are studied, as well as its mild reduction to the C3-aminoalkylazetidinol motif found in the anti-cancer drug cobimetinib.

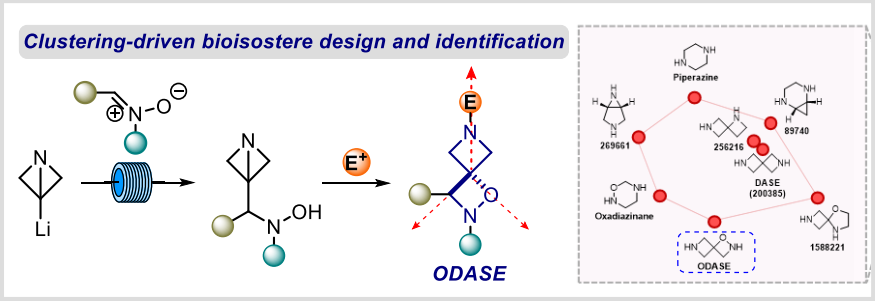

Figure 1: ODASE as a novel bioisostere

Acknowledgements: We thank the University of Bari for support. This project has received funding from the European Union's Horizon Europe under the Marie Skłodowska-Curie action MSCA-PF, grant agreement ExpandFlow No. 101106497. This work was supported by the Italian MUR under the framework of the Action IV.6 PON R&I 2014-2020 – DM 1062. Prof. E. Schingaro is acknowledged for the use of the Single Crystal X-ray Facility at the Department of Earth and Geoenvironmental Sciences, University of Bari. Thanks are also due to Dr. Tobias Stürzer (Bruker AXS) and Prof. Michele Zema (University of Bari) for the low-temperature X-ray data collection in Karlsruhe, Germany.

Keywords: *azabicyclo[1.1.0]butane, flow chemistry, bioisostere, strained spiro heterocycle, azetidine*

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Spectroscopy-based metabolomics for early detection of *Citrus Tristeza Virus* infection

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Metabolomics is a powerful tool for studying various aspects of plant physiology and biology, which regulate plant growth, development, and stress response. To protect themselves from pathogens, plants produce a wide range of secondary metabolites through a network of different biosynthetic pathways. The analysis of metabolomic data allows the identification of groups of metabolites, whose concentration significantly changes already at the first stages of disease. Metabolomics can be utilized as a tool to detect host-pathogen interaction and also to differentiate the type of compounds produced in resistant and susceptible phenotypes.[1] Recently, our lab has been involved in a number of projects based on the application of spectroscopy-based metabolomics for the study of plant diseases, including *Erwinia amylovora* infections in pear[2] and *Xylella fastidiosa* infections in olive crops.[3,4] Furthermore, some important clues on the resistance phenomenon against *Xylella fastidiosa* were obtained by investigating the composition of the xylem sap of plant species characterized by a different phenotype towards Xf subspecies pauca.[5]

This study focuses on *Citrus Tristeza Virus* (CTV) infections in citrus trees. CTV is the causal agent of "tristeza", one of the most destructive viral diseases of citrus. The CTV is phloem-limited and its transmission into new geographic areas occurs by the introduction of infected plants or budwood, with subsequent local dispersal in a semi-persistent mode by several aphid species.[6] In this study, a combined approach by nuclear magnetic resonance (NMR) and hyperspectral reflectance (HSR) spectroscopies is used. NMR is the most robust and non-destructive technique for the elucidation of unknown compounds: as it is not selective, it allows for an unbiased view of the chemical composition of the sample. HSR provides a rapid detection tool, requires limited sample preparation, and is a non-invasive technique for plant disease detection.

Among the objectives of the present study is the identification of possible biomarkers of CTV infection by NMR and subsequent correlation with specific HSR wavelengths. The latter can be advantageously exploited for the development of sensors for the early detection of CTV infections.

Keywords: *metabolomics; nuclear magnetic resonance (NMR); hyperspectral reflectance (HSR); early detection*

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Lignin valorisation for biofuel and chemicals production

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Lignin, a key component of plant biomass, has great potential as a sustainable resource for bioenergy and bioproducts. Its abundance and renewability make it a promising alternative to fossil fuels.[1] Deep Eutectic Solvents (DES) are effective green solvents for breaking down lignin, facilitating its conversion into valuable chemicals.[2] Additionally, nickel-based catalysts, such as Raney-Nickel, are highly effective in depolymerizing lignin, especially in electrocatalytic hydrogenolysis, making the process more efficient and sustainable.[3] This study demonstrates that the hydrogenation of lignin using Nickel Raney catalyst is highly dependent on the reaction conditions. The optimal conditions were identified, providing the highest yield and selectivity of depolymerized products. While the oil production percentage remained stable between methanol and ethanol, using higher amounts of Nickel Raney led to the formation of eicosane, demonstrating the potential for producing alkanes. Raising the reaction temperature decreased the amount of phenolic compounds but increased the production of esters and aromatic compounds. These findings offer valuable insights for efficiently converting lignin into valuable chemical feedstocks, contributing to the development of sustainable biomass utilization strategies.

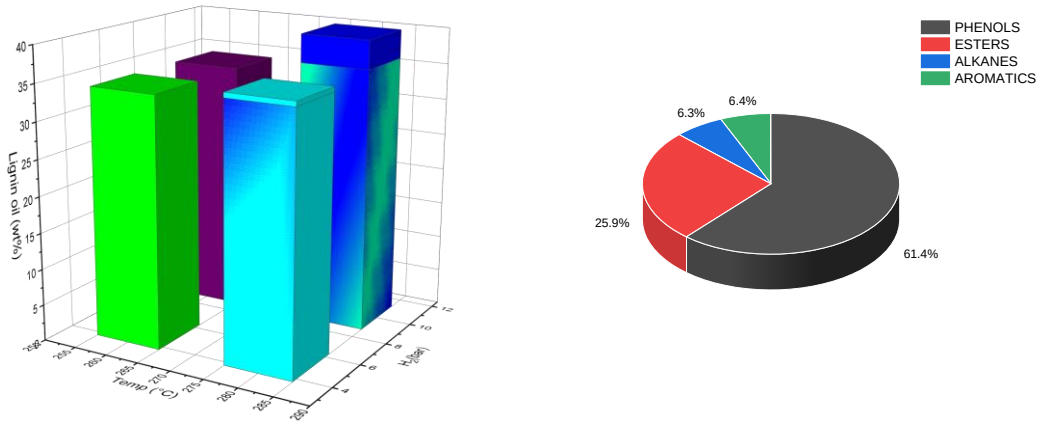

Figure 1: A) Lignin oil yield conversion in the presence of different amounts of Raney-Nickel, 80 and 200 mg. All reactions proceeded for 4 hours B) Product distribution

Acknowledgements: We appreciate the support of the ENEA Research Institute for providing funding(fellowship) and resources.

Keywords: *Lignin, Valorisation, Catalyst*

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Towards sustainable materials and chemicals: extraction and characterization of mucilage polysaccharides from *Opuntia-ficus indica*

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In the last twenty years, many researchers in several fields have shown more and more interest in *Opuntia* species of plants. Their goal was the identification and isolation of compounds that could represent innovative and useful resources in various sectors. Many studies focused on *Opuntia ficus-indica*, which proved to be an excellent candidate as a source of raw materials, highlighting its potential to play a role in industries 1. This work presents an investigation aimed to characterize aqueous extracts from *O. ficus-indica* cladodes (*O. ficus-indica* stems), focusing on their content in specific classes of compounds and functional groups. The ATR-FTIR difference spectroscopy was successfully applied for this purpose.

A modified protocol 2 to isolate the mucilage fraction of *O. ficus-indica* was employed and its efficiency was assessed based on the thermal pre-treatment of the raw biomass. The extraction yield was evaluated as extract mass per dry weight of cladodes, ranging from 37.0 mg/g to 46.2 mg/g.

The ATR-FTIR analysis was carried out on lyophilised extracts both as powders and resuspended in water. The IR spectra outlined the presence of functional groups referred to the target polysaccharides, suggesting that the extraction protocol was effective in isolating mucilage. Furthermore, the protonation-induced difference spectroscopy 3 allowed to detect a high content in carboxylic functional groups, which can be referred either to anionic polysaccharides or to low molecular weight organic acids coming from *O. ficus-indica* metabolism. Finally, Folin-Ciocâlteu and ABTS-decolorization assays were carried out to evaluate the polyphenol content and the antioxidant capacity of the extracts.

Though preliminary, our results encourage further studies, aiming to unveil the potential of these *O. ficus-indica* biocompounds in several fields, such as the production of biocoatings for food, sustainable concrete, biofuel, and even for wastewater treatment.

Keywords: *Opuntia ficus-indica, FTIR-ATR spectroscopy, cladodes, mucilage.*

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Natural Deep Eutectic Solvents and Ultrasound-Assisted Extraction (NADEs-UAE): A Novel Approach for Polyphenol Extraction from Endemic Apulian *Salicornia europaea* L.

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Salicornia europaea L., commonly known as sea asparagus or glasswort, is an edible plant with a tuberous, succulent, hairless, and leafy stem, highly branched with distinct joints. Salicornia species are halophyte plants, well adapted to saline environments and found along the coasts of Europe, America and Asia.

This study explores the optimization of polyphenol extraction using Natural Deep Eutectic Solvents (NADEs) and ultrasound-assisted extraction (UAE). The tips of *S. europaea* were collected from the Apulian Adriatic coast, dried for 48 hours at 40°C, and then ground into small particles with a diameter of 200 µm. A software-based prediction method (BIOVIA COSMOtherm - Dassault Systèmes, Paris, France) was used to select solvents that act as hydrogen bond acceptors (HBA) and donors (HBD) for polyphenol extraction from *S. europaea*. Six different NADEs were synthesized at 50°C for 2 hours, and polyphenol extraction was then performed in an ultrasonic bath at 30°C for 30 minutes. An aqueous-alcoholic mixture (1:1) served as the control under the same UAE conditions. Four chemical assays, including Folin-Ciocalteau, DPPH, ABTS, and FRAP, were conducted to evaluate the total polyphenol content (TPC) and antioxidant activity of the *S. europaea* NADEs extracts. Additionally, the stability of TPC was monitored over a 3-month period. The most promising TPC result, 6.08 ± 0.06 mg GAE/g dry weight, was obtained using proline (HBA) and malic acid (HBD). Regarding the antioxidant assays, the most promising results were obtained from proline:malic acid and choline chloride:urea NADEs mixtures, with IC_{50} values of 0.05 and 0.09 mg GAE/g dry weight, respectively. The TPC results monitored over three months revealed choline chloride:urea, citric acid:glucose, and proline:malic acid mixtures as the most stable over time.

The results highlight the significant advantages of using this NADEs-UAE approach, which might be directly applied in food, nutraceutical, and pharmaceutical products, bypassing purification processes.

Keywords: *Salicornia, extraction, NADEs, polyphenols*

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Determination of volatile organic compounds (VOCs) in indoor work environments by solid phase microextraction-gas chromatography-mass spectrometry

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Volatile Organic Compounds (VOCs) are emitted into the atmosphere from natural and anthropogenic sources. It is therefore imperative to study these compounds and monitor them effectively, through the development of reliable methods[1,2]. In this study, an untargeted volatolomic approach is proposed for the evaluation of occupational exposure to volatile organic compounds (VOCs) of workers in an engine manufacturing plant in Southern Italy. The study of indoor working environment conditions was conducted in a variety of areas and at different stages of the work process, with the objective of assessing the respective risks. The degree of occupational exposure to VOCs was determined by GC-MS measurements coupled with Head-Space Solid-Phase Microextraction (HS-SPME). The analytical procedure was optimized in terms of SPME fiber type used, time allowed for adsorption, time allowed for desorption, and temperature gradient. In order to extract the volatile organic compounds (VOCs), the SPME fibers were exposed to the headspace in two distinct areas of the manufacturing facility: the mixing and painting chamber and the engine painting area. Furthermore, the sampling was conducted with the painting system in operational state (system on) and with the painting system deactivated (system off). In total, 212 compounds were identified, but only 17 were consistently present in both zones (the mixing painting chamber and engine painting area), regardless of system conditions (on or off). Finally, a semi-quantitative evaluation was performed, considering the peak area value of the most toxic compounds, by multivariate data analyses (ANOVA and Principal Component Analysis), to explore differences in the VOC composition.

Keywords: Indoor air quality, Industrial emissions , Solid phase microextraction (SPME), Gas chromatography-mass spectrometry (GC–MS)

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PK/PD of imipridone-based mitochondrial *h*ClpP activators

Anselma Liturri, Morena Miciaccia, Domenico Armenise, Olga Maria Baldelli, Mariachiara Mammone, Giovanni Graziano, Marialessandra Contino, Savina Ferorelli, Antonio Scilimati, Maria Grazia Perrone

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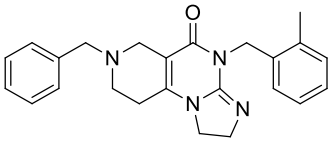
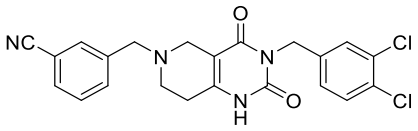
Human caseinolytic protease P (*h*ClpP) is a tetradecamer serine protease, involved in the mitochondrial proteastasis. *h*ClpP catalyzes the hydrolysis of misfolded and damaged proteins recognized by ClpX, forming with ClpP the soluble complex ClpXP. *h*ClpP is upregulated in many primary and metastatic human tumors thus representing an intriguing therapeutic target.[1]

ONC201 has been identified as an allosteric activator of *h*ClpP (*h*ClpP EC_{50}= 5.90±0.42) and proposed as a treatment for high-grade glioma being also able to cross the blood-brain barrier[2]. However, its pharmacokinetic profile requires optimization. This led to a new class of *h*ClpP activators, the TR derivatives, including THX6, endowed with a meaningful pharmacological effect.[3]

THX6 has been tested as *h*ClpP activator (*h*ClpP EC_{50}= 1.18±0.14), cytotoxic in several tumor cell lines and to determine oxidative damage in increased reactive oxygen species (ROS) production model.



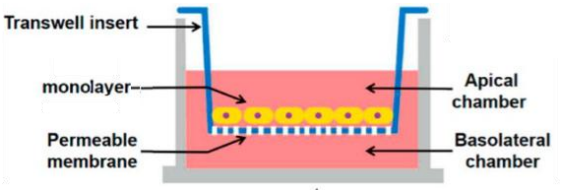
ONC201



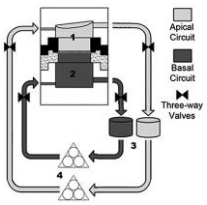
THX6

To predict intestinal and brain penetration, pharmacokinetic properties were investigated by studying THX6 interactions with efflux pumps and measuring its permeability across Caco-2 and MDCK-MDR1 cell monolayer in millicell transwell system.

Static condition



Dynamic condition



Moreover, to better mimic the *in vivo* environment, a new dynamic permeability assay has been developed by using LiveBox2 bioreactor (IVTech), which represents a 5D dynamic model. The results of such experiments will be presented.

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Keywords: *hClpp, ONC201, pharmacokinetic profile, in vitro assay.*

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Advancing Tin-Based Perovskite Solar Cells: Interface Engineering with Chelating Agents for Enhanced Stability and Performance

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Perovskite solar cells (PSCs) have emerged as promising candidates for next-generation photovoltaic devices due to their high-power conversion efficiency and solution-processable fabrication. However, their widespread adoption faces a significant challenge: the reliance on lead-based materials in stable perovskite formulations, which often contain more than 30% lead by weight[1]. Lead is a well-documented toxic metal associated with severe environmental contamination and adverse health effects, including neurological and developmental damage in humans[2]. Its presence in PSCs raises concerns about potential risks, particularly during fabrication and device operation[2]. Tin-based perovskites, such as $FASnI_3$, present a promising alternative due to their low bandgap, large charge-carrier mobility, and low exciton binding energy[3] which could enable competitive power conversion efficiency (PCE), and stability compared to their lead-based counterparts[1]. Despite their potential, tin-based perovskites face significant challenges, with stability being the most critical. When Sn^{2+} is used to replace Pb^{2+} at the B position of the ABX_3 perovskite lattice, a significant increase in electronic defects and the consequent doping level within the perovskite film is systematically reported and dramatically impacts the device's PCE[1]. A critical mechanism behind forming electronic defects is the oxidation of Sn^{2+} to Sn^{4+} during the deposition of the perovskite film. Solvent systems play a critical role in controlling these processes. While dimethyl sulfoxide (DMSO) aids in film uniformity, it accelerates Sn^{2+} oxidation[1]. Alternative solvent systems, such as a combination of diethylformamide (DEF) and 1,3-Dimethyl-3,4,5,6-tetrahydro-2(1*H*)-pyrimidinone
(DMPU) in a 6:1 volume ratio, have demonstrated improved performance in $FASnI_3$ film preparation[4].
In this work, we address another critical aspect of stability: the interface between the perovskite layer and charge transport layers (HTL/ETL). We investigated various additives acting as chelating agents for tin-based ions and performed DFT calculations to identify the chelating complex most selective toward Sn^{4+}. This selectivity could play a crucial role in preventing tin oxidation, thereby enhancing the stability and efficiency of the corresponding solar cells. Furthermore, this approach underscores the potential of interface engineering and tailored chelators to advance the performance of lead-free perovskite solar cells.

Keywords: *tin perovskite solar cells, chelating agents, interface engineering*

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In vitro validation of cannabinoid receptor subtype 2 (CB2R) selective fluorescent probes SM15 and VM7

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The cannabinoid receptor subtype 2 (CB2R), together with subtype 1 (CB1R), is a key component of the endocannabinoidome (eCBome). While CB2R is physiologically mainly peripherally located, it becomes overexpressed in certain inflammation-based diseases, such as neurodegenerative diseases and cancer[1,2]. This evidence makes CB2R an emerging pivotal biomarker to identify the first steps of inflammation-based diseases such as cancer and neurodegeneration. To deepen the knowledge of the CB2R pathways impacting the onset of the above-mentioned pathologies, we designed a series of fluorescent ligands spanning from the green to the near-infrared (NIR) regions of the light spectrum[3,4], to address the need for green and safe alternatives to the commonly used radiative technologies. Among the fluorescent ligands synthesized in our laboratory, compounds **SM15** and **VM7**, both bearing a *N*-Adamantyl-4-oxo-1,4-dihydroquinolinone scaffold, exhibited a favorable CB2R pharmacodynamic profile (good affinity and high selectivity towards CB2R). **SM15** and **VM7** have been validated in flow cytometry assays (fluo-saturation and fluo-competition binding experiments) and in fluorescent microscopy. Noteworthy, **VM7** has been successfully used to detect in vitro microglia cells mimicking inflammation states where CB2R are overexpressed.

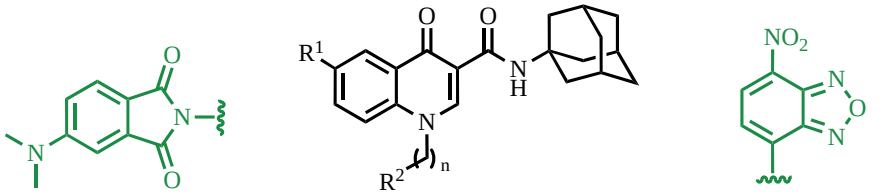

Figure 1: Fluorescent ligands scaffold and fluorescent moieties structure

Acknowledgements: The authors gratefully thank NextGeneration EU_PNRR_M4.C2 Investimento 1.1._PRIN-P2022TRR3Y- AID-CARE Funding.

Keywords: *Cannabinoid receptor, CB2R, inflammation, fluorescent probes*

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Green recovery of high value-added products from shrimp wastes for a sustainable economy

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Better management of fish waste and the recovery and valorisation of discarded biomass are important steps to facilitate the transition to a circular economy, which will reduce the environmental impact caused by the landfilling of this waste and maximise its commercial value.

This study focuses on the valorisation of red shrimp shells, provided by a local fish company, which are rich in astaxanthin (AXT), a xanthophyll with a high antioxidant activity[1], and chitin, a biopolymer with various properties and applications. Natural Deep Eutectic Solvents (NADES)[2] were used as alternative to conventional solvents, ensuring sustainability standards during the whole extraction process. In particular, hydrophobic NADES, composed of menthol and alkanoic acids in a 1:1 molar ratio, were successfully applied for AXT extraction. The extraction method was optimised by changing various parameters and operating conditions, resulting in a fast, safe and economical process. The bioactivity of AXT extracts was assessed by measuring the Trolox Equivalent Antioxidant Capacity (TEAC). With a view to a commercial product based on AXT extracted from shrimp wastes, the use of α-cyclodextrin as an emulsifier to create NADES/water emulsions was considered, improving the stability over time and the dispersibility in water of the hydrophobic AXT extracts, thus paving the way for further in-vitro toxicity and bioactivity tests. Moreover, the remaining AXT extraction byproduct was used to isolate chitin by a hydrophilic NADES based on choline chloride and lactic acid in a 1:1 molar ratio. This NADES effectively dissolved calcium carbonate and lowered the protein content of chitin fibers, allowing to get a raw chitin product in a single step without the need for mineral acids and strong bases.

Acknowledgements: This research was granted by Action IV.4 PON for Research and Innovation 2014-2020.

Keywords: Astaxanthin, DES, shrimp wastes, circular economy

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Source Apportionment of Real-Time Ultrafine Particulate Matter in a Mediterranean Urban Center During the Summer

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Increase in human activities within urban centers in recent years has resulted in an increase in the number of individuals exposed to progressively higher levels of atmospheric pollutants such as particulate matter. An increasing number of studies demonstrates the significance, for public health scopes, of characterizing not only the total mass of particulate matter but also studying the size distribution of particles and attributing their sources. Although there have been efforts to normalize the particulate emissions in PM10 and PM2.5 fractions, little has been done for the ultrafine fraction, which constitutes the majority of total particle number concentrations (PNCs). The aim of this study is to characterize the emission sources affecting the urban center of Lecce (Italy), which is representative of medium-sized cities in terms of urban planning and climate, during the summer period.

The sampling site is located at "Piazza Ludovico Ariosto"-Lecce, where the main sources of airborne particulate matter are vehicular traffic, biomass combustion from human activities, regional background, and dust transport from the saharan region. A total of 39 days were sampled using a real-time AQ-SMART 1000 (PALAS) station, which analyzes particles using an optical analyzer based on the Light Scattering principle (spectral analysis), wich can provide real-time particle number and size class distribution. Continuous 1-minute observations were obtained for each of the 64 size classes, covering a range from 0.175 µm to 18 µm, and mass concentrations of PM1, PM2.5, and PM10.

The data were then processed to obtain daily averages of PM1, PM2.5, and PM10 masses and their respective ratios PM2.5/PM10, PM1/PM10, and PM1/PM2.5, which allowed us to identify a Saharan Dust event confirmed by back trajectories and satellite images, and some days characterized mainly by ultrafine particulate matter attributable to anthropogenic sources such as vehicular traffic. Next, data on the number of particles for different size classes were considered, and Positive Matrix Factorization (PMF)[1] was applied to confirm the emissive sources impacting the urban center of Lecce, including vehicular traffic, regional background, and Saharan dust.

Assigning a size range of atmospheric particulate matter to a specific source provides a helpful tool for decision makers, enabling them to implement effective and sustainable solutions to improve air quality and the health of urban residents.

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Synthesis of Aza-S(VI) Fluorides and Primary Sulfonimidamides from Sulfinylamines

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Aza-S(VI) fluorides are gaining increasing importance in assembling pharmaceutically relevant compounds due to their electrophilic properties facilitating the formation of S-O, S-N and S-C bonds.[1,2] Whereas sulfonyl fluorides have been widely explored, their aza-isosters represent a viable alternative due to the substitution of the oxygen atom with an NH group, which improves physico-chemical properties.[3] In this context, sulfonimidoyl fluorides and sulfondiimidoyl fluorides, have been less explored due to lengthy sequences which often require the generation of more reactive intermediate such as aza-S (VI) chloride[4] or the use of harmful gaseous reagents.[5] Considering the potential application of these compounds in the development of innovative pharmacophores and the current limitations in their synthesis, we developed a fast one-pot method for the synthesis of sulfonimidoyl fluorides from sulfinyl amines by nucleophilic addition of organometallic reagents and electrophilic fluorination mediated by NFSI.[6] An analogous sequence has been used for the synthesis of sulfondiimidoyl fluorides by the formation of the sulfurdiimide from the corresponding sulfinyl amine. Furthermore, we explored the reactivity of aza-S(VI) fluorides via fluorine exchange with different nucleophiles, providing an efficient methodology for the synthesis of various aza-S(VI) fluorides compounds.

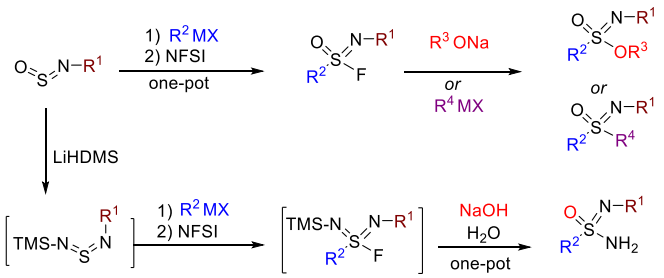

Figure 1. One-pot preparation of sulfonimidoyl fluorides and sulfonimidamides from sulfinyl amines

Acknowledgements: We thank the University of Bari for support. We are grateful to Mr. Domenico Cellamare for technical support.

Keywords: *Sulfonimidoyl fluorides; Sulfondiimidoyl fluorides; Sulfonimidamides; Sulfinylamines*

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Electrochemical and spectroscopical characterization of apta-sensor based on poly-L-Dopa modified gold electrodes

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The development of new biotechnological integrated and miniaturized devices is an interesting aspect of biosensors application in different biomedicine fields, for example for detection of pathogenic microorganisms, such as *Listeria monocytogenes*, able in contaminating food. The fast and easy detection of a particular target is the aim of these kinds of new biosensors, which promise to be easy to use and reproducible portable devices. In this work, gold screen printed electrodes (SPEs) are modified by electrochemical deposition of a polymer, which works as a linker for an aptamer that acts as *bait* for detection of target protein of interest. The biosensor in question wants to be suitable for detection of Internalin A (InlA) surface protein of *Listeria m*. To functionalize this biosensor, L-Dopa polymer is used, a chiral amino acid known for its adhesive properties [1]. Then, a specific aptamer for InlA is drop-casted onto modified electrode, where its -NH_2 group exploits polymer free functional groups to adhere on working electrode. Each functionalization step has been characterized by electrochemical techniques, performing Cyclic Voltammetry (CV) and Electrochemical Impedance Spectroscopy (EIS) in $[Fe(CN)_6]^{3-/4-}$. To appreciate polymerized L-Dopa characteristic groups, Infrared (IR) and Raman Spectroscopies were also performed.

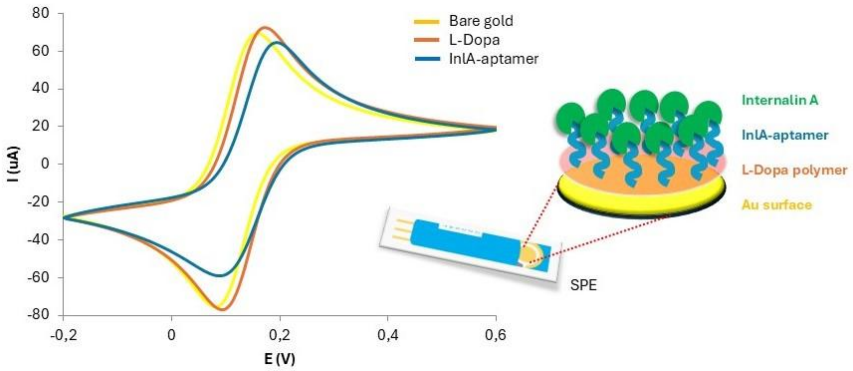

Figure 1: Graphical scheme of modified SPE with a CV performed in $[Fe(CN)_6]^{3-/4-}$.

Acknowledgements: The authors acknowledge the support of the European Union by the Next Generation EU project PRIN2022 – 2022JRKETK_PE7 - Versatile hybrid in-fiBer Optical-electrocHemical systEMs for wIdely Applicable bioseNsing – BOHEMIAN.

Keywords: *Aptamers; Biosensors; Electroanalysis; Electro-polymers.*

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Engineering ceria nanoparticles to improve the performance of biohybrid microbial photoelectrodes

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Bio-electrochemical systems (BES) are an innovative approach to sustainable energy production, leveraging biological catalysts such as enzymes, organelles, and bacteria. Among these, photosynthetic bacteria are particularly compelling due to their ability to facilitate biohybrid photoelectrochemical systems for solar-to-electrical energy conversion[1]. However, their practical application is hindered by challenges such as limited solar light absorption, inefficient extracellular electron transfer (EET), and low stability under operational conditions[2,3]. To address these limitations, this study explores the integration of engineered nanomaterials with bacterial cells, focusing on cerium oxide (CeO_2) nanoparticles functionalized with diverse groups (citrate, aspartate) to enhance microbial-electrode interactions. Specifically, CeO_2 nanoparticles were designed to reduce the impact of reactive oxygen species (ROS)[4], which induce oxidative stress and compromise the stability of biohybrid systems. Our study builds on previous work that demonstrated enhanced current generation through the modification of the purple photosynthetic bacterium Rhodobacter capsulatus (*R. Capsulatus*) with cysteine-functionalized gold nanoparticles[5]. By complementing this strategy with ROS-scavenging CeO_2 nanoparticles, it is possible to achieve further stabilization of the biohybrid microbial photoelectrodes. This underscores the potential of such variously functionalized nanomaterials in advancing BES technology, specially in overcoming biological and electrochemical limitations, hence contributing to the development of sustainable bioenergy solutions.

Keywords: *Bio-electrochemical systems, cerium oxide, R. capsulatus, sustainable*

Acknowledgements: The authors want to acknowledge for financial support the European Union through Next Generation EU, Mission 4 Component1, from Ministery of University and Research within PRIN call 2022 PNRR Photocatalytically regenerable hierarchically porous adsorbents for efficient water treatment PHOTOPAD, P2022FP2W4, 2023-2025CUP B53D23027540001

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Extraction and purification of antimicrobial peptides and their adsorption on mesoporous silica nanoparticles

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Histatin 5 and 6 (H5/H6) are peptides with a very high antifungal activity against *Candida albicans*, a pathogenic yeast responsible for infections involving, among others, the gastrointestinal trait and oral cavity.[1] The aim of this work is to carry out the purification of H5/H6 extracted from human saliva and the adsorption on mesoporous silica nanoparticles (MSN)[2] to obtain an antifungal drug delivery system. MSN and amino functionalized MSN (MSN-NH_2) samples were synthesized and fully characterized through several physico-chemical techniques (e.g. SAXS, TEM, N_2-adsorption isotherms, ATR-FTIR, DLS, ELS and TGA). The extracted H5/H6 samples were purified by mean of the protocol proposed by Flona et al.[3] which includes the use of HPLC. The good outcome of purification was qualitatively tested through HPLC combined with mass spectrometry (HPLC-MS). The H5/H6 peptides, dissolved in a 10 mM Tris-HCl buffer solution at pH 7, were physically adsorbed both on MSN and MSN-NH_2. The loading of the peptide, quantified through a bicinchoninic acid assay, was higher on the bare MSN rather than on MSN-NH_2 (8487 ± 84 µg/g vs 4216 ± 76 µg/g, respectively). These results can be rationalized in terms of intermolecular interactions among the peptides and the bare/functionalized MSN surface. Indeed, at pH 7, the peptides are positively charged (IEP ~ 10), hence attractive electrostatic and van der Waals interactions are expected with the negatively charged silica surface, whereas repulsive electrostatic forces, but still attractive van der Waals interactions, will occur with the positively charged amine groups of MSN-NH_2.

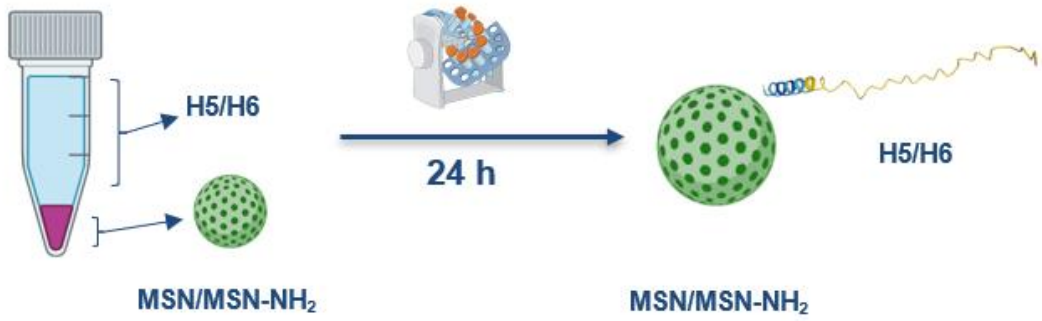

Figure 1: H5/H6 adsorption experiment on MSN/MSN-NH_2 (image created with Biorender.com)

Keywords: *histatin 5/6, drug delivery, MSN, adsorption*

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Nanostructured cathodes functionalized with redox molecules for energy storage

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Lithium-ion rechargeable batteries are the main power source for portable devices, such as mobile phones and other electronics.[1,2] Their demand is rapidly increasing due to the growth of the consumer electronics market.[3]However, the dependence on non-renewable materials such as cobalt raises concerns about the sustainability of future reserves.[4] Organic materials represent a promising alternative to inorganic counterparts, [5] with quinones standing out due to their high theoretical charge capacities and the possibility of modulating the redox potential through specific functional groups.[6,7] This project aims to overcome the limitations of organic-based cathodes by developing hybrid electrodes with redox molecules covalently attached to semiconductor nanostructures. This approach reduces the solubility of the active species in the electrolyte, enhances the efficiency of the redox reactions at the electrode/electrolyte interface and increases the specific capacity thanks to the high surface area of the nanostructures. Different semiconductors (ITO, SnO_2, TiO_2) are investigated in order to identify the most suitable material in terms of chemical stability, energy level alignment and charge transfer efficiency, with the ultimate goal of optimizing the overall performance of the device.

Acknowledgements: The author gratefully acknowledges support from the European Research Council (ERC), ERC Consolidator Grant ''HYNANOSTORE" (project number 101045746), from the European Union –NextGenerationEU, the National Recovery and Resilience Plan (NRRP), Project code PE0000021, "Network 4 Energy Sustainable Transition –NEST" – CUP B53C22004060006 and from the PRIN PNRR 2020 HEROES (cod. P2022AFYZX)

Keywords: Nanostructured cathodes, Organic molecules, Eco-sustainable batteries, Hybrid Electrodes

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Structural Implications of Missense Point Mutations in SBDS: Insights from a combined SAXS/MD investigation

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[Ω]G.M. and V.N. contributed equally to this study

Shwachman-Diamond syndrome (SDS) is a rare autosomal recessive disorder characterized by pancreatic insufficiency, skeletal abnormalities, and bone marrow dysfunction, with an increased risk of myelodysplastic syndrome and leukaemia. This study combines comparative molecular dynamics (MD) simulations and Small-Angle X-ray Scattering (SAXS) to study the Shwachman-Bodian-Diamond syndrome protein (SBDS). We investigate the molecular basis of the syndrome by examining conformational dynamics change of a set of missense mutants of SBDS compared to its wild type. Our observations suggest that different mutations may impact (i) the interaction of SBDS with the ribosome, (ii) the binding of SBDS to EFL1, and (iii) the SBDS rearrangement coupled to EFL1 binding. Extensive MD simulations, with a total simulation time of 13 μs, revealed variations in the interdomain flexibility of SBDS, consistent with previously published affinity data and SAXS experimental data presented here. We propose a structural rationale behind the previously reported weakened interaction of mutants I167T, R175W, and I212T with EFL1. Additionally, our SAXS data indicate that R19Q, I167T, and R175W mutants exhibit altered relative abundances of SBDS conformational states in solution, corroborating the computational results. Overall, our integrated computational and experimental approach provides a comprehensive understanding of how specific mutations in SBDS alter its structural dynamics and binding interactions.

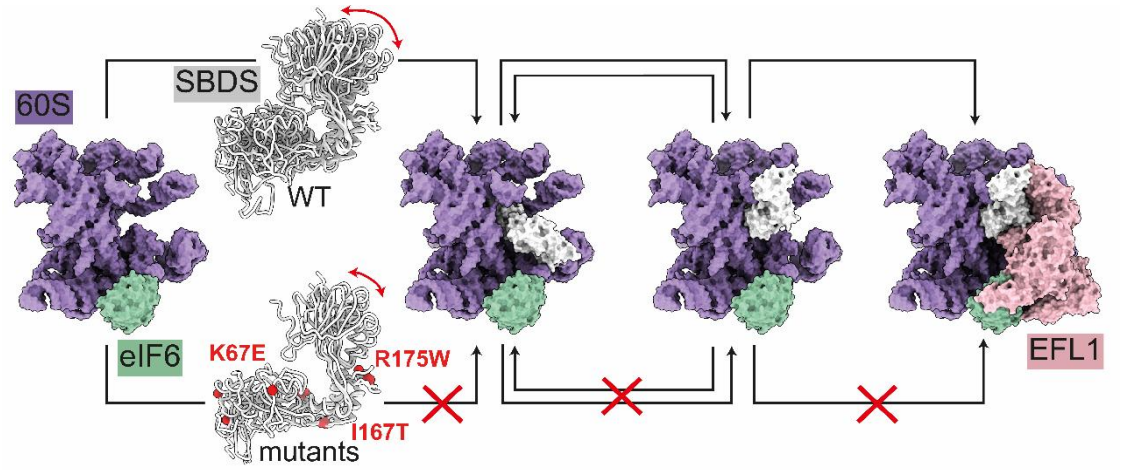

Figure 1: SBDS point mutations interfere with the maturation process of the ribosome 60S subunit.

Keywords: *Schwachman-Bodian-Diamond syndrome protein, Molecular Dynamics, Small-Angle X-ray Stattering, Disease-causing mutations*

Waste Treatment and Disposal Plant: evaluation of emission impact and air quality

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Humans can distinguish millions of colors and nearly half a million tones, but the number of identifiable odors remains unknown. Odors pose significant environmental challenges for industries like water treatment, waste disposal, livestock farming, and catering. While no direct health impacts from odor nuisances have been proven, they cause persistent discomfort for nearby residents, potentially leading to conflicts. Odor responses are categorized as 'bottom-up' or 'top-down'[2] and influence both existing operations and site selection for new facilities. This project aims to establish a scientific basis for developing standards on odor measurement and limits for emissions from waste treatment plants.

From May 2024 measurement of odorous have been carried out by using innovative sensors placed upstream (PA1) and downstream (PA2) the landfill area (Figure1). The pollutants measured were ammonia (NH_3) and hydrogen sulphide (H_2S), primarily generated by waste degradation.

Preliminary results collected from June to August 2024 showed higher NH_3 and H_2S levels at PA2, possibly due to nearby agricultural activities. Weak winds (~9 m/s) and 60% relative humidity contributed to poor ventilation and pollutant buildup at PA2.

Although pollutant levels remained below regulatory limits, the Odor Index (OI), reflecting the cumulative perception threshold of detected compounds, was significantly higher at PA2 (~0.8), indicating a potential olfactory impact. Further analyses are planned to explore seasonal variability, environmental sources, and long-term trends. The results of the present work will improve monitoring plan and network with advanced sensors and odor mitigation techniques.

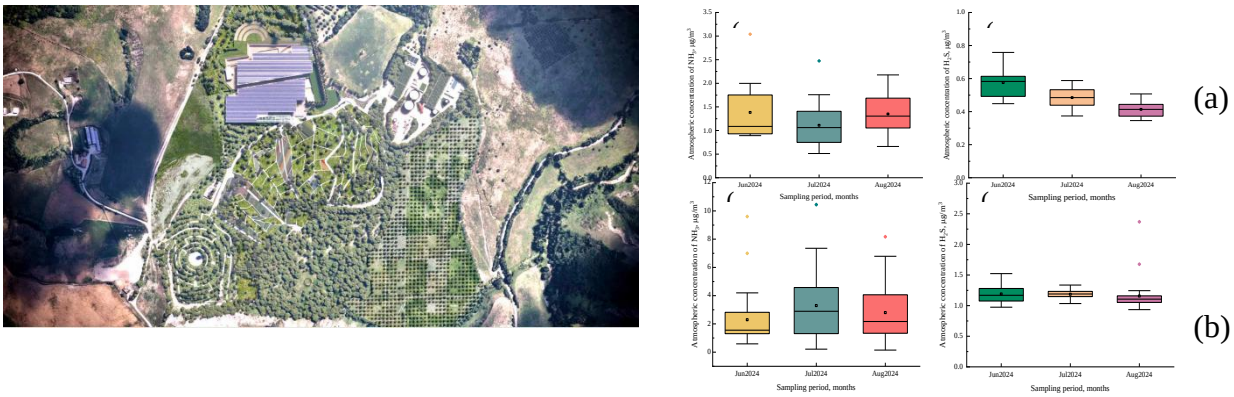

Figure 1: Map of the landfill and summer evolution of the atmospheric concentrations of NH_3 and H_2S measured at the two sampling points PA1 (a) and PA2 (b)

Keywords: *Odours, Pollutants, Measurement, Legislation*

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LC-MS characterization of allergens released by innovative food packaging

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The growing interest in recent years in the ecological transition has led to new materials, including novel biocompatible food packaging based on naturally available substances such as alginate, soya, or a mixture of different components[1]. These new materials may raise concerns about the potential release of allergenic proteins from the packaging to food during its storage. The allergens are usually proteins that can trigger an adverse reaction in sensitive people, from milder forms, such as skin rashes, to more severe forms, such as anaphylaxis[2]. The European Union with Regulation No. 1169/2011 has identified 14 allergenic ingredients, including milk, soya, eggs, peanuts, crustaceans, nuts, fish, cereals containing gluten, molluscs, celery, mustard, sesame, lupine and sulphur dioxide. In recent years, new allergens are also emerging related to novel foods, such as algae and insects[3]. This study focuses on an innovative food packaging based on a zein-casein film. In detail, 3% (w/v) of caseins is added to improve the mechanical properties of the film based on zein. Caseins, known allergenic milk proteins, can potentially migrate into food; therefore, their release must be evaluated to protect the health of sensitive individuals. In this work, we aimed at characterizing the aqueous extracts from zein/casein films focusing specifically on allergenic proteins and their release into different food simulants.The aqueous extracts are digested with trypsin and analysed by matrix-assisted desorption/ionization (MALDI)-time-of-flight (TOF)/TOF mass spectrometry (MS) and by reversed-phase liquid chromatography (RPLC) coupled with high/low resolution MS. Our strategy clearly identified the marker peptides corresponding to different caseins, such as FFVAPFPEVFGK at *m/z* 692.869^{2+} for *α*-S1, NAVPITPTLNR at *m/z* 598.343^{2+} for *α*-S2, AVPYPQR at *m/z* 415.729^{2+} for *β* and YIPIQYVLSR at *m/z* 626.358^{2+} for *κ*-casein. These peptides were monitored to quantify the protein releases in three simulants mimicking foods. At a preliminary stage, an innovative industrial alginate-based packaging has also been studied to search for the presence of residual potential allergenic proteins as contaminants of the alginate and their possible release in foodstuffs. First results indicate the absence of algal proteins or peptides in alginate bulk biopolymer.

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Keywords: allergens, food packaging, mass spectrometry

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In vitro bio-characterization of Mesoporous Silica Nanoparticles for controlled Deferoxamine delivery

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Neurodegenerative diseases (ND) have brain dysregulated metal homeostasis. This disfunction contributes to the generation of reactive oxygen species, neuronal damage and promotes the formation of toxic protein aggregates. Following convincing scientific evidence that metals are involved in the pathogenesis of ND, metal chelators are being studied as promising treatments against these disorders. Deferoxamine (DFO) is an FDA approved drug used for the treatment of iron overload and appears to have great potential observed in preclinical studies involving ND. However, DFO has a particularly short plasma life (20-90 min), so to ensure its effectiveness, high doses should be administered to the patient for 5-7 days per week. This systemic treatment raises concerns about its toxicity. Thus, it is essential to develop new DFO formulations to overcome these limits[1,2].

In this context, Mesoporous Silica Nanoparticles (MSNs) have attracted significant attention as drug delivery systems (DDS) due to their unique properties, their high surface area and large volume pore enable efficient loading of drug candidates. MSNs have, in addition, excellent biocompatibility and stability, ensuring no toxicity and low total clearance rate[3].

Drug-Structure-Directing Agent (DSDA) is a new synthetic method to produce DDS. It consists in the use of molecules with pharmacological activity as template to generate MSNs.

In vitro biological characterization data of DFO@MSNs synthesized using the DSDA methodology will be presented.

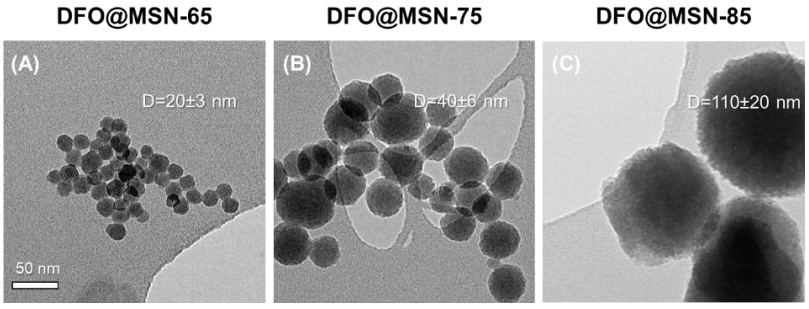

Figure 1: TEM images of DFO@MSNs produced by varying the reaction temperature: (A) 65°C, (B) 75 °C and (C) 85 °C.

Keywords: MSN, deferoxamine, neurodegenerative diseases.

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Deep Eutectic Solvents for New Low Environmental Impact Methodologies for Polymer Waste Transformation

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Polymeric materials play a ubiquitous role in nearly every facet of human activity owing to their remarkable chemical and mechanical resilience. However, their exceptional properties come at a cost, most polymers are notoriously non-biodegradable, posing a significant ecological challenge due to their persistent accumulation in the biosphere.

In recent years, substantial efforts have been directed towards reducing plastic consumption and enhancing chemical recycling methods[1]. Yet, there remains a pressing need for innovative green technologies to address the recovery, treatment, and chemical recycling of polymer waste. This would enable their transformation into reusable raw materials or high-value products. Among the myriad thermoplastic polymers utilized in daily life and plastic manufacturing, polyethylene terephthalate (PET) and polyurethane (PU) stand out as both prevalent and environmentally detrimental pollutants.

Our research is committed to developing greener and more environmentally sustainable depolymerization techniques as viable alternatives to conventional processes. To this end, we are exploring the application of Deep Eutectic Solvents (DES) or their aqueous solutions as reaction media for plastic depolymerization. These solvents offer favourable chemical and physical properties, ease of production and utilization, and recyclability[2].

In this communication, we present our findings on DES-promoted depolymerization of PET and PUs chains, enabling the monomers recovery as new raw building blocks to be used in the synthesis of other new polymers or fine chemicals. This represents a crucial step towards a more sustainable approach to polymer waste management and resource utilization.

Acknowledgements: This research work was funded by Ministero dell'Università e della Ricerca (MIUR) through the PRIN project "REPLAY" (2020SBNHLH_003), Ministero dell'Ambiente e della Sicurezza Energetica (MASE, ex MITE) through the project "GreenChemBioDEP" (H93C22000380001), and by the Apulian Regional Project "Green Chemistry and Biocatalysis for the development of new low environmentally friendly methodologies for the transformation of polymer waste" (996968a3) "Programma Regionale RIPARTI" POC PUGLIA FESR-FSE 2014/2020.

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Nature-inspired design of new anti-Alzheimer's multi-target drugs: the NInFA project

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Alzheimer's disease (AD) is one of the most common causes of dementia in the elderly with a major impact on the economy and healthcare, affecting about 50 million patients worldwide[1-3]. It is characterized by an unknown origin and absence of effective treatments. In fact, the few available drugs can only improve symptoms with a low impact on the progression of the disease[1-3].

Several hypotheses have been proposed to describe the complex AD physiopathology suggesting the multi-target paradigm as a promising approach to discover new potential anti-AD drugs[1].

Since the nature has always been considered as an important source inspiration for the discovery and development of drugs, natural scaffolds can be used as starting point for the design of new anti-Alzheimer agents with innovative profiles[1]. Then, starting from recently published results[2,3], new nature-inspired molecules have been designed in silico within the activity planned in the framework of the recently funded project NInFA [4].

These molecules will be obtained by a semisynthetic approach combining fungal secondary metabolites (ochratoxin α, OTα and/or ochratoxin β, OTβ) with different synthetic moieties able to mimic some of the few drugs currently available for the therapy of AD. The different synthetic pathways will be optimized in the framework of green chemistry, in particular by using Deep eutectic solvents, alcoholic media or neat conditions. Lastly, their potential anti-AD activity will be evaluated through biological assays performed on classical and innovative targets of AD.

In this communication, preliminary results of both synthesis and production/extraction activities will be discussed.

Acknowledgements: Finanziato dall'Unione europea- Next Generation EU, Missione 4 Componente 1 CUP: H53D23007940001

Keywords: Alzheimer's disease, Multi-Target, Semisynthesis, Green Chemistry

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Lipidomic analysis of edible insects by LC-MS

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As the global population increases, edible insects are emerging as a viable alternative to traditional foods due to their high content of proteins, vitamins, minerals, and lipids [1]. Entomophagy, the practice of consuming insects, is common in Africa, Asia, and South America but remains relatively rare in Western countries. Edible insects are not only consumed as food but are also used in supplements and gluten-free products to enhance the chemical, physical, and sensory qualities of food items. To minimize bacterial contamination, deactivate degradative enzymes, and extend the shelf-life of these foods [2], processing techniques like pasteurization, roasting, and drying are crucial. However, these processes can impact the nutritional content of these foodstuffs. For instance, heating can initiate the Maillard reaction, which involves the amino groups of phosphatidylethanolamines (PEs) [3] resulting in the generation of modified compounds. This study focuses on the lipidomic characterization of modified PEs in *Acheta domesticus* (house cricket), a species suitable for human consumption, using high-resolution mass spectrometry (HRMS) coupled with liquid chromatography (LC). Both hydrophilic interaction liquid chromatography (HILIC) and reversed-phase liquid chromatography (RPLC) coupled with electrospray ionization (ESI)-HRMS were employed. This approach enabled the identification of conventional phosphoglycerolipid classes, as well as modified PEs, most likely formed through the Maillard reaction. Several modified PEs were identified, including *formyl-PE* (FPE), *acetyl-PE* (AcPE), *hydroxymethylfurfurenyl-PE* (HMF-PE), and *Amadori glycation products* (AmPE and LacPE) resulting from non-enzymatic lipid glycation. To better understand the interaction between the glycosidic group and the amino functionality of PEs, in-vitro reactions were conducted using standard PEs and isotopically labelled glucose ($^{13}C_2C_4H_{12}O_6$). The identification of these modified lipid classes appears promising, as their presence seems to be associated with oxidative stress processes and the pathophysiology of diseases such as Alzheimer's and type 2 diabetes [4-5].

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Keywords: *Lipidomics, LC-MS, Insect, PEs.*

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Oxidative Potential of Particulate Matter: new multi-sample analysis protocol

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The study of oxidative potential of particulate matter (PM) is a key element in understanding its potential adverse effects on biological systems. Acellular assays help indicate the ability of PM to produce reactive oxygen species, which are associated with cellular damage and oxidative stress, providing useful information on health risks. The aim of this work is to optimise the analytical protocols of two acellular assays: the dithiothreitol (DTT) assay and the ascorbic acid (AA) assay for the estimation of oxidative potential, in order to optimise the classical methodology reported in the literature[1,2].

$PM_{2.5}$ samples were collected in the Lecce area as part of the TOX-IN-AIR project and analysed using different analytical techniques to obtain information on the chemical composition of PM. A quarter of the PM filter was subjected to DTT and AA assays using a Fluostar Omega multi-plate reader equipped with auto-injectors. This methodology has proven effective, allowing the extension of these tests to a larger number of samples due to its ability to reduce sample volume requirements and analysis time, while simultaneously improving the reproducibility and standardization of measurements. Currently, no standard analysis method exists for these assays. In this context, the use of an automated instrument can help to reduce operator-related uncertainties and provide a more accurate estimate of the oxidative potential of particulate matter.

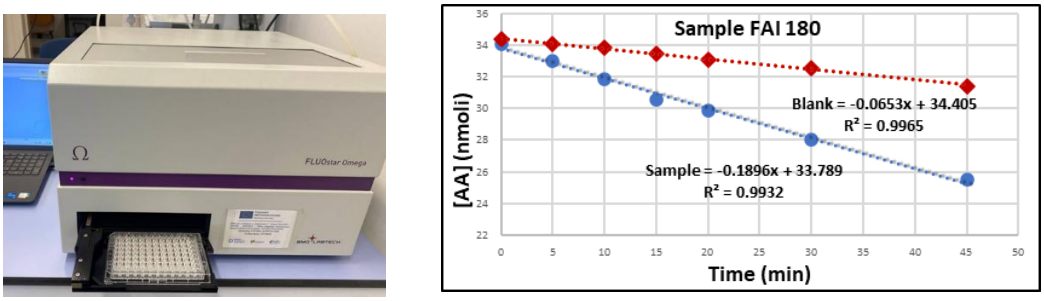

Figure 1: Multi-plate reader Fluostar Omega; Analysis of a real sample using AA assay.

Acknowledgements: The study was carried out within the framework of the project "TOX-IN-AIR - Funded by the European Union Next Generation EU, Call PRIN 2022 PNRR - Project P2022JKP2S, PNRR, Mission 4, Component C2, Investment 1.1."

Keywords: *Particulate Matter; Oxidative Potential, Air pollution.*

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Design and synthesis of a bicyclic peptide analogue of the β-sheet domain of arc repressor

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ARC repressor is a transcription factor belonging to ribbon-helix-helix family: its dimeric unit is able to bind to a specific sequence of DNA and to control gene expression, through the β-sheet domain. The aim of this project is the design, synthesis and characterization of a bicyclic peptidic analoque of the β-sheet domain of arc repressor. Starting from the native sequence of the β-sheet, a bicyclic analogue made of 16 aminoacids has been designed. The purpose is to mimic a β-hairpin structure by binding, to both β-strands, a D-Pro-L-Pro template that could act as a β-turn and induce a proper folding of the linear structure, in order to form a hairpin[1]. In this structure, the two β-strands are antiparallel and mimic the native β-sheet domain (Figure 1).The linear structure of the peptide was synthesized via Solid Phase Peptide Synthesis (SPPS), carried out on 2-chlorotrityl chloride resin, using Fmoc-aminoacids with protected side chains. Macrocyclization was conducted through a coupling reaction via Liquid Phase Peptide Synthesis (LPPS)[2]. The formation of the disulphide bridge has been obtained through an oxidation with iodine, in solution. Further structural investigation and binding essays are in progress, in order to confirm the correct folding of the peptide and its ability to bind to DNA.

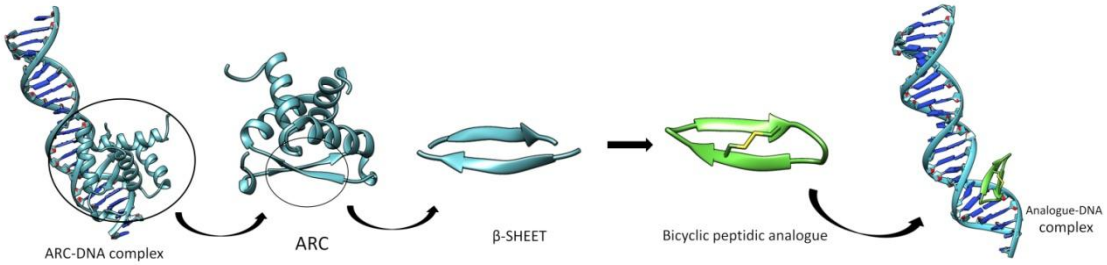

Figure 1: Design of the synthetic analogue of the β-sheet domain of ARC.
These images have been prepared using UCSF Chimera1.16 (https://www.cgl.ucsf.edu/chimera/).

Acknowledgements: We acknowledge financial support under the National Recovery and Resilience Plan (PNRR), Mission 4, Component C2, Investment 1.1, Call for tender No. 1409 published on 14.9.2022 by the Italian Ministry of University and Research (MUR), funded by the European Union – NextGenerationEU– Project TitleUltrasonic Technology for the Sustainable Chemical Synthesis of Peptide-based Therapeutics (US4PepTher)-CUP D53D23016950001- Grant Assignment Decree No. 0001384 adopted on 01-09-2023 by the Italian Ministry of Ministry of University and Research (MUR).

Keywords: arc, peptides, synthesis, resin

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Cellulose-based nanostructured aerogels for leachate decontamination: towards sustainable phosphorus recovery from sewage sludge ash

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Recent data from the European Union classify phosphorus as a critical raw material. Efficient methods for recovering phosphorus (P) from sewage sludge ash through wet chemical extraction followed by precipitation have been developed, with the primary challenge being the co-dissolution of metals along with P from the ash[1].

In this study, we propose an effective and sustainable strategy for decontaminating leachate derived from sewage sludge ash using eco-friendly cellulose-based nanostructured aerogels (CNS). These aerogels are synthesized via the 2,2,6,6-Tetramethylpiperidin-1-yl)oxyl (TEMPO) oxidation of cotton-derived cellulose, followed by ultrasonication and thermal cross-linking with branched polyethylenimine (bPEI)[2]. We conducted lab-scale adsorption tests with varying amounts of CNS (1, 3, and 10 g_{CNS}/L), both in the presence and absence of citric acid (10 g/L), across a pH range of 1.5 to 10. The concentrations of phosphorus and metals (As, Cu, Cr, Ni, Zn, Fe, Al) were monitored during these tests. After decontamination, phosphorus was precipitated from the leachate using $Ca(OH)_2$ to reach the desired pH (Figure 1).

The results demonstrated that the CNS were effective in adsorbing significant quantities of metallic ions, particularly Fe and Al, reducing their concentrations by 40% and 30%, respectively, under strongly acidic conditions. The solid precipitate obtained at pH 8 from the decontaminated leachate (after adding 10 $g_{citric\ acid}$/L and 10 g_{CNS}/L) met the requirements set by EU regulation 2019/1009 regarding P_2O_5 and heavy metals, indicating its potential for use as a raw material in the production of inorganic fertilizers[3].

Figure 1: Leachate decontamination process to recover sustainable phosphorous.

Acknowledgements: This study was carried out within the PNRR RETURN Extended Partnership.

Keywords: *Cellulose-based sorbents, Circular economy, Sustainable fertilizers*

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Advanced biosensors for early detection of clinically relevant biomarkers

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The valuable market of In-vitro diagnostic (IVD) is mostly driven by the prevalence of infectious and chronic diseases as well as the increasing demand for point-of-care (POC) diagnostics.[1] For instance, there is a huge request for cost-effective screening methods for those virus infections that can produce cancer states. High-risk Human Papilloma Virus (HPV) infection is a well-established cause of cervical cancer and a relevant factor in other anogenital and head-neck cancers.[2] Indeed, cervical cancer is estimated to cause 341,831 deaths globally each year, with 9/10 deaths occurring in developing countries. The availability of POC testing for fast mass-screening and early identification of infected hosts is fundamental for timely and effective therapies.

The study herein proposed is focused on the development of a bio-electronic portable platform, namely the Single Molecule with a large Transistor (SiMoT),[3] for the early detection of clinically relevant biomarkers. The focus is on the validation of a standardized protocol for the definition of the diagnostic sensitivity and selectivity of the bioelectronic device and on the applicability of the platform for the ultra-sensitive immunoassay of HPV capsid proteins at the limit of identification (LOI). The work aims to the rapid screening of viral targets in plasma and vaginal swabs, using a few µ-litres of diluted bio-fluids collected from 200 patients.

The study foresees the biofunctionalization of the SiMoT disposable cartridge with capturing antibodies or probes for the selective HPV assay. The sensing measurements are processed using machine learning approaches to obtain a reliable response and a fully digital output. The high selectivity and sensitivity of the bio-electronic sensor would guarantee false positives and false negatives to be below 1%.[4,5] Also, to prove the competitiveness of the SiMoT platform, the performances will be compared with gold standards based on PCR technology. Starting from the experimental evidence already achieved with the SiMoT technology in relevant environments (Technology Readiness Level, TRL 5), the study aims to bring the proposed platform to the demonstration of the early assay of HPV infection in real samples collected at least from 200 patients (TRL 6 pre-clinical evaluation phase).

Acknowledgments: We acknowledge partial financial support by: The Complementary National Plan PNC-I.1 "Research initiatives for innovative technologies and pathways in the health and welfare sector" D.D. 931 of 06/06/2022 DARE - DigitAl lifelong pRevEntion initiative (code PNC0000002, CUP: B53C22006420001); and "Centro di Innovazione Regionale" Digital Assay, Regione PUGLIA Delibera Regionale n 702 del 08/11/2022 (CUP B93C22000840001).

Keywords: biomarker early-detection, biosensors, immunoassay.

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Development of Synthetic Polymers as Sustainable Release Agents

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Release agents play a key role in modifying the peeling strength of a removable carrier layer from a solid support substrate (**figure 1**). The chemical composition of the release layer must be opportunely tuned in a way to ensure compatibility with the carrier material while maintaining a sufficiently weak interfacial bond to the substrate. Under these conditions, the carrier along with the release layer can be cleanly stripped away from the finished product.[1] One of the widely employed natural release agents is carnauba wax. Unfortunately, its chemical composition is affected by a significant variability across production batches, which adversely affects formulation consistency and alters its physicochemical properties as a release material.

a. b.

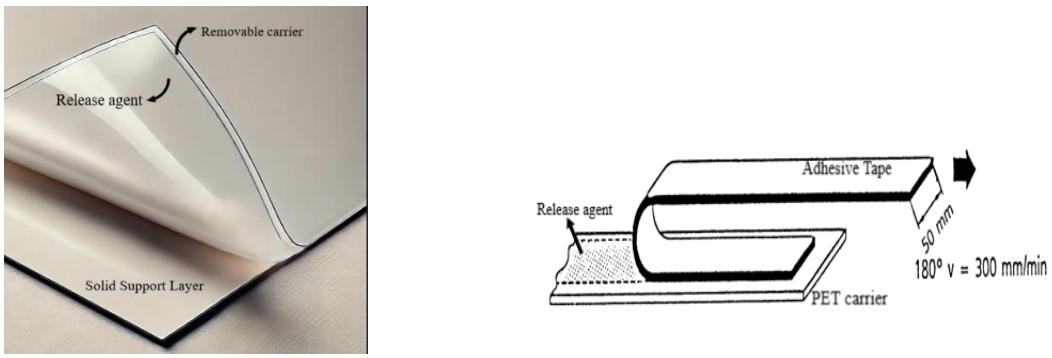

Figure 1: a) Scheme of a typical multilayer system consisting of support substrate, release and carrier. b) Scheme of a standard peeling-test.

Our project is focused on the development of innovative materials to be included as release agents in composite products, including the synthesis of new polymeric materials and the development of their formulations in accordance with the requirements of Health, Safety, and Environment.[2] New polymers showing useful functional features such as improved mechanical properties, are synthesized and, thus, exploited for innovative composite products. Formulation studies are performed on the prepared polymers. During the research activity, a special focus is on the principles of eco-design and green chemistry, looking at the ecological and toxicity profile of the reagents and solvents used. The synthesized materials were fully characterized through chromatographic, thermal, and spectroscopic analyses. Besides, their performance as release agents was assessed through peeling-adhesion tests. The results of this study support the development of new polymer synthesis strategies to modulate adhesion properties while maintaining solubility in green solvents, thus promoting sustainability in industrial applications. In the present communication, the objectives and the main milestones of the conducted research activities will be described.

Keywords: release polymers, peelable coatings, green solvents, composite materials

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Ag_3PO_4-based nanostructures for antimicrobial coatings

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Antimicrobial effects of silver nanomaterials have been studied throughout history. However, nano-safety concerns have been recently raised on their use, especially when their diameter is below 20 nm [1]. For this reason, part of the scientific community working on nano-antimicrobials is currently focused on developing new antimicrobial materials that could be eco-friendly and less toxic. In this context, silver phosphate emerges as a promising candidate. Some studies showed how this salt can be effective against bacteria as *E. coli, S. aureus* [2] and fungi such as *C. albicans* [3]. Specifically, silver phosphate can generate reactive oxygen species (ROS) upon excitation by visible light [4]. Furthermore, Ag_3PO_4 has a limited solubility in water (0.02 g/L at 25 °C) and as such if provides a way to control the release of Ag^+ ions, which exhibit a well-known antimicrobial activity [5]. In addition, compared to other insoluble silver salts, such as halides, sulphide, etc., Ag_3PO_4 has the advantage of releasing phosphate anions, which are not dangerous for human health. In this communication, the development of bioactive coatings based on silver phosphate microparticles is proposed. Ag_3PO_4 particles were synthesized following a modified version of the precipitation method formerly proposed by Wang et. al.. Hybrid zinc phosphate and silver phosphate materials were developed as well, with the perspective of reaching a synergistic antimicrobial effect of the two metallic cations. As a preliminary experiment to develop antimicrobial coatings, both the Ag_3PO_4 nanostructures and the hybrid Ag^+-Zn^{2+} material was embedded in a polyvinyl alcohol polymeric matrix (PVA). PVA was chosen since it is a biocompatible and non-toxic polymer commonly used in the food packaging industry. The details of the synthesis and the analytical characterizations (infrared and X-ray photoelectron spectroscopy, electron microscopy) will be presented. The chemical composition and morphology of the developed materials will be discussed and correlated to the application perspectives.

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Keywords: Antimicrobial, Silver Phosphate, Zinc Phosphate, Co-precipitation.

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Quantitative and Non Targeted NMR Approaches in Metrological Traceability

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NMR spectroscopy is gaining increasing importance in analytical chemistry. In the last decade, quantitative NMR (qNMR) and untargeted approaches have enabled great improvements in both the quantification of molecules in complex mixtures and the identification of product characteristics in suitable sample pools. Metrological traceability of products can be successfully achieved by qNMR even when certified reference materials are not commercially available. Along with the quantification and purity assessment of molecules, NMR is also emerging as a powerful tool in food chemistry, especially when looking for product characteristics such as cultivar, geographical origin, typicality of the production process, etc.

The great application potential of NMR spectroscopy arises from the fact that, according to theory, the ratio of a signal generated by the molecule under investigation to the signal of a reference molecule depends exclusively on the corresponding molar ratio. In other words, when a given sample is analyzed by different spectrometers, the same output in terms of signal ratios is obtained regardless of the hardware configuration. This offers a unique opportunity to develop analytical systems capable of identifying sample characteristics and quantifying several molecules [1,2,3]. In particular, the case study of both the identification of wheat and pasta samples and the quantification of betaine will be presented. The advantages and limitations of using non targeted NMR analyses performed at different magnetic fields will also be discussed.

Keywords: *NMR spectroscopy, Food analysis, Metrological Traceability.*

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LC-MS Profiling of Bioactive Compounds from Agricultural By-products for Pharmaceutical and Biofuel Applications

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In the context of the National Operational Program (PON) Project, this study explores the valorization of agricultural and food by-products as a sustainable source to extract bio-compounds with potential applications in pharmaceutical and biofuel industries. In the framework of this project, the recovery and characterization of several bioactive molecules have been afforded from diverse biomass sources, including lignified pistachio1 and walnut2,3 shells, tomato by-products4, and Kombu brown algae5.

Pistachio shells were found to be a rich source of anacardic acids (AnAs), a class of secondary metabolites with promising health benefits. Notably, positional isomers of AnAs with alkyl chains 15:1 (Δ8 and Δ6) and 17:1 (Δ10 and Δ8) were identified for the first time, opening new avenues for the systematic study of their bioactivities1.

Walnut shells, often discarded as waste, revealed high concentrations of ellagitannins and phenolic compounds. Among the ellagitannins, compounds with complex structures such as mono-, di-, tri-, tetra-, and pentagalloyl glucopyranoses were detected, along with those featuring hexahydroxydiphenoyl (HHDP) groups, with antioxidant properties and potential health-promoting applications in pharmaceutical and cosmetic formulations. The intricate diversity of these compounds, characterized by more than 10 isomers in some cases, underscores challenges in definitive structural identification2. Additionally, fatty acid analysis showed the presence of unsaturated species such as FA 18:2 (Δ9,12) and FA 18:3 (Δ9,12,15), which contribute to the nutritional and bioenergetic value of these extracts3.

In tomato by-products, L-NAPEs (Lyso-N-acyl phosphatidylethanolamines) were identified as important lipid species, after setting a robust method to distinguish them from phosphatidylethanolamines4. Finally, rare aminophospholipids (Phosphatidyl-O-[N-(2-Hydroxyethyl)Glycine], PHEGs) were isolated from kombu seaweed, with the most abundant species identified as PHEG 20:4/20:4 and its hydroxylated derivatives5.

These findings underscore the significance of advanced analytical approaches, including liquid chromatography and high-resolution mass spectrometry, to elucidate complex molecular profiles. The exploration of these secondary metabolites, particularly ellagitannins, fatty acids, and lipids with unique structural features, not only supports waste reutilization but also contributes to a circular bioeconomy.

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Reshaping Ritter Reaction in Deep Eutectic Solvents: Sustainable Synthesis of Amides

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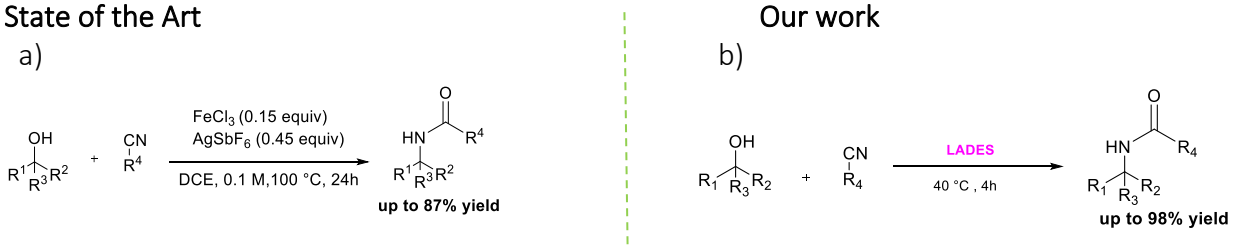
Amides are fundamental compounds in chemistry, showcasing a vast spectrum of applications across biology, medicine, chemical synthesis, and material sciences [1]. Among the numerous synthetic methodologies available, the Ritter reaction, first introduced by John J. Ritter in 1948 [2], has emerged as one of the most significant and versatile approaches for the production of amides. Traditionally, the Ritter reaction has relied on harsh reaction conditions, including the use of strong acids (e.g., trifluoromethanesulfonic acid) [3], harmful inorganic catalysts (e.g., $CoCl_2$) [4], toxic and volatile organic solvents (e.g., dichloromethane) [5], reactive anhydrides (e.g., propyl phosphonic anhydride) [6], and high temperatures (Figure 1a) [7]. These factors not only pose significant safety risks but also conflict with the principles of sustainable chemistry. In this communication, we present a **green and efficient procedure** for the synthesis of amides under mild and environmentally benign conditions. The process leverages **Lewis acidic deep eutectic solvents (LADESs),** which act simultaneously as catalysts and solvents (Figure 1b). This innovative approach enables the transformation of secondary and tertiary alcohols into amides by reacting them with both aliphatic and aromatic nitriles. The method achieves excellent yields of up to 98%, under mild conditions (40 °C, 4 h), without requiring column chromatography for product purification.



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Keywords: *Ritter reaction, Amides, Lewis acidic deep eutectic solvents*

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Natural urease inhibitors from lignocellulose

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Urea is the main source of N in worldwide crop production, but its rapid hydrolysis catalysed by soil urease resulted in a substantial decrease in fertilisation efficiency. Also, the rising pH impacts plant germination or early growth. Overall, the main problem remains ammonia volatilization, considering the compound itself and contributing to atmospheric pollution by reacting with acid pollutants (e.g., SO_2, NO_x)[1]. Using urease inhibitors as N-stabilizers has been implemented to counterbalance these negative aspects. One of the most used for agronomic purposes is N-(n-butyl) thiophosphoric triamide (NBPT), often co-formulated with urea for a controlled release of both the fertilizer and the urease inhibitor. Catechol and catechol-like molecules have been widely studied as alternatives but many of these compounds have safety issues[1].

In the present work, different aromatic molecules obtainable from lignocelluloses were investigated to understand any possible structure-activity regarding urease inhibition and find sustainable and safe substitutes for commercial urease inhibitors.

The inhibition experiments were performed on Jack bean urease as well as urease naturally present in soil samples. Preliminary results indicate that the phenolic compounds here tested have a wide range of inhibition activity (from 2 to 48%) but no one of them reach the performance of catechol. The best inhibition results were obtained with a bio-oil obtained by pyrolysis of wood at 650°C and 2,6-dimethoxyphenol (Figure 1).

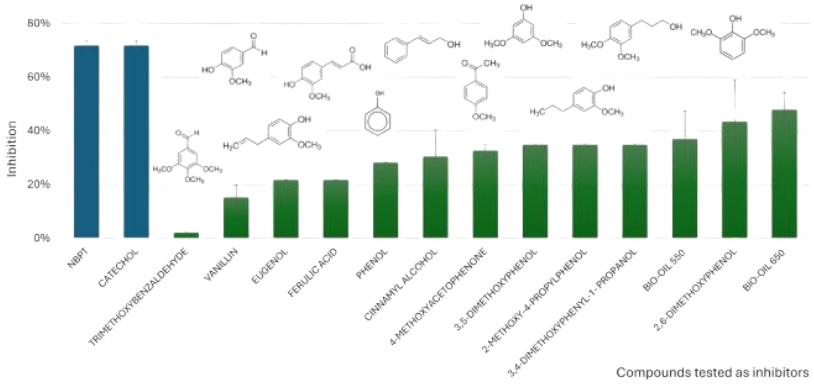

Figure 3. Inhibition of the activity of soil urease achieved by various aromatic compounds, in comparison to NBPT and catechol.

Keyword: *urea, soils, ammonia, environment.*

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