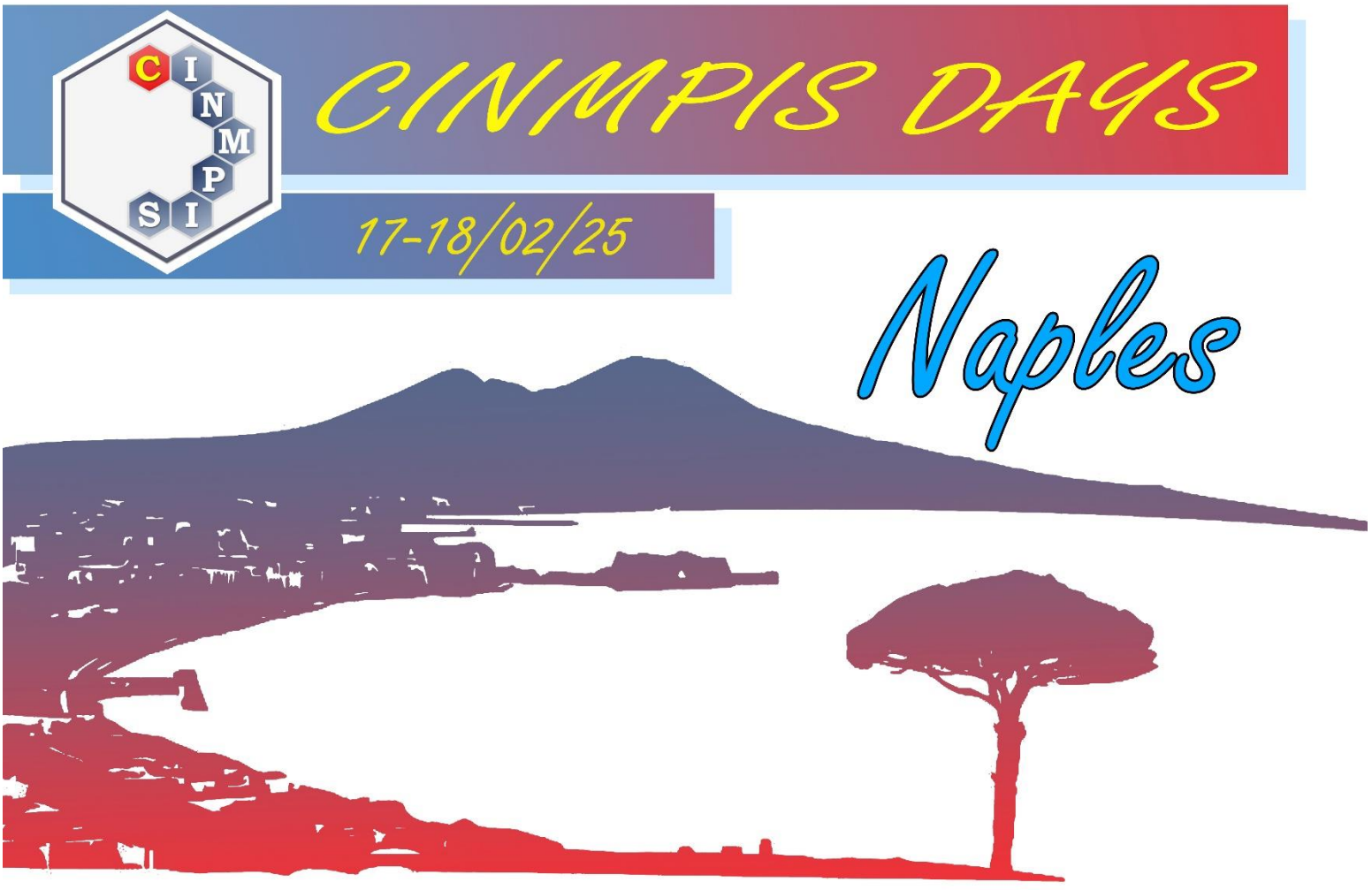
Consorzio **I**nteruniversitario **N**azionale
Metodologie e **P**rocessi **I**nnovativi di **S**intesi (**CINMPIS**)

XXIII GIORNATE SCIENTIFICHE
DEL CONSORZIO CINMPIS

CINMPIS DAYS 2025

17-18 February 2025

Centro Congressi, Università di Napoli Federico II,
via Partenope 36, Napoli



CINMPIS associated universities:

Università di Bari Aldo Moro

Università della Basilicata

Alma Mater Studiorum - Università di Bologna

Università di Cagliari

Università della Calabria

Università di Camerino

Università di Catania

Università di Messina

Università di Milano-Bicocca

Università di Napoli Federico II

Università di Pavia

Università di Perugia

Università di Pisa

With 2025, the CINMPIS Days proudly reach their XXIII edition, reaffirming their role as a premier scientific conference organized by the National Interuniversity Consortium for "Innovative Synthetic Methodologies and Processes" (CINMPIS Consortium). This annual event has established itself as a pivotal forum for the advancement of chemical synthesis, bringing together leading Italian and international scientists. The program features *Plenary Lectures*, *Keynote Lectures*, and *Oral Communications* delivered by distinguished experts, alongside *Flash Presentations* showcasing the work of emerging young researchers.

The CINMPIS Consortium serves as a dynamic scientific network dedicated to fostering knowledge, driving innovation, and promoting technology transfer across all domains of chemical synthesis. Headquartered at the University of Bari "Aldo Moro", **CINMPIS currently includes 13 Italian universities**—Bari, Basilicata, Bologna, Calabria, Cagliari, Camerino, Catania, Messina, Milano-Bicocca, Napoli Federico II, Pavia, Perugia, and Pisa. The Consortium is also set to expand further, with the Universities of L'Aquila, Salerno, and Torino soon becoming part of its growing network!

CINMPIS DAYS 2025 are organized by the University of Napoli Federico II, thanks to the collaborative effort of its Departments of *Chemical Sciences*, *Pharmacy*, *Physics*, and *Molecular Medicine and Medical Biotechnologies*. Through the years, this conference has become an essential meeting point for academics and industry professionals working in the field of chemical synthesis, fostering synergies that drive scientific progress and innovation. Founded in 1994, the CINMPIS Consortium (www.cinmpis.it) now includes **over 350 professors and researchers**, spanning a diverse range of expertise. The Consortium's multidisciplinary approach encompasses regio- and stereoselective synthesis of bioactive compounds for applications in biomedicine, agriculture, food science, and drug discovery, as well as advancements in green chemistry, biotechnologies, and the development of innovative organic materials for opto-electronic applications.
The ***Plenary Lectures*** at CINMPIS DAYS 2025 will be delivered by Prof. **M. Carmen Galan** (University of Bristol, UK) – *CINMPIS Lecturer* – and Prof. **Maurizio Prato** (CIC bioMAGUNE, San Sebastian, Spagna, formerly University of Trieste). The ***Keynote Lectures*** will be given by a distinguished panel of speakers: Proff. **Luca Beverina** (University of Milano-Bicocca), **Sergio Mauricio Bonesi** (University of Buenos Aires), **Giancarlo Cravotto** (University of Torino), **Leonardo Degennaro** (University of Bari), **Carmine Gaeta** (University of Salerno), **Giuseppe Gattuso** (University of Messina), **Andrea Gualandi** (University of Bologna), **Loredana Maiuolo** (University of Calabria), **Enrico Marcantoni** (University of Camerino), **Domenica Musumeci** (University of Napoli Federico II), **Alessandra Operamolla** (University of Pisa), **Daniele Passarella** (University of Milano Statale), **Simona Riela** (University of Catania), **Giuseppe Sforazzini** (University of Cagliari). Additionally, **two special *Keynote Lectures*** will be delivered by the **CINMPIS 2024 Prizewinners**: Prof. **Alessandro Palmieri** (University of Camerino, *Prize for Innovation in Organic Synthesis*) and Dr. **Giulia Brufani** (University of Perugia, *Prize for the Best PhD Thesis*). The scientific program will be further enriched by 25 *Oral Communications* and 19 *Flash Presentations*. Further details are available on the official conference website: *www.cinmpis2025.it*.

On behalf of the Board of Directors of the CINMPIS Consortium, I extend my sincere gratitude to the *Organizing Committee* of the University of Napoli Federico II, with special thanks to Prof. Daniela Montesarchio, Chair of the conference, and the entire Team whose dedication has been instrumental in ensuring the success of this event, which welcomed over 140 participants! A heartfelt appreciation also goes to Mr. Carlo Gianeselli of the CINMPIS Consortium for his invaluable support. Finally, my deepest and most heartfelt gratitude to all participants, speakers, and session chairs for their enthusiasm and commitment. Thanks for helping make CINMPIS DAYS 2025 a truly exceptional and inspiring event!

Looking forward to welcoming you in Napoli!

Prof. Vito Capriati
Director of CINMPIS Consortium *Napoli, February 17, 2025*

SPONSORS:

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CINMPIS days - Previous editions:

I **Pavia**, October 9, **2001** (University of Pavia)

II **L'Aquila**, October 28, **2002** (DOMPE′ SpA)

III **Lecce**, September 18-19, **2003** (University of Lecce)

IV **Firenze**, October 22, **2004** (University of Firenze)

V **Bari**, November 7, **2005** (University of Bari)

VI **Bologna**, October 13, **2006** (University of Bologna)

VII **Napoli**, November 29, **2007** (University of Napoli Federico II)

VIII **Milano**, November 25, **2008** (University Statale di Milano)

IX **Padova**, September 2, **2009** (Complesso San Gaetano)

X **San Benedetto** (AP), September 17, **2010** (Convention Center "PalaRiviera")

XI **Bari**, November 25, **2011** (University of Bari)

XII **Milano,** December 3, **2012** (University of Milano-Bicocca)

XIII **Perugia**, December 18, **2013** (University of Perugia)

XIV **Bari**, September 29-30, **2014**, Ventennium Conference (Univ. of Bari)

XV **Napoli**, December 11-12, **2015** (University of Napoli Federico II)

XVI **Rende**, December 16-17, **2016** (University of Calabria)

XVII **Cagliari**, December 15-16, **2017** (University of Cagliari)

XVIII **Bologna**, February 18-19, **2019** (University of Bologna)

XIX **Pavia**, February 20-21, **2020** (University of Pavia)

XX **Messina**, September 7-8, **2021** (University of Messina)

XXI **Pisa**, February 9-11, **2023** (University of Pisa)

XXII **Bari**, February 7-9, **2024** (University of Bari)

CINMPIS Lecturers:

CINMPIS Lecturer 2012 Prof. Ilan Marek, Technion – Istrael Institute of Technology, Haifa, Israel

CINMPIS Lecturer 2015: Prof. Bernd Plietker, University of Stuttgart, Germany

CINMPIS Lecturer 2017: Prof. Dieter Seebach, ETH Zürich, Switzerland

CINMPIS Lecturer 2018: Prof. Dr. Syuzanna R. Harutyunyan, University of Groningen, Netherlands

CINMPIS Lecturer 2019: Prof. Karl Anker Jørgensen, Aarhus University, Denmark

CINMPIS Lecturer 2021: Prof. M. Carmen Carreño, Madrid Autonomous University, Spain

CINMPIS Lecturer 2022: Prof. Darren J. Dixon, University of Oxford, UK

CINMPIS Lecturer 2023: Prof. Helma Wennemers, ETH Zürich, Switzerland

CINMPIS Lecturer 2024: Prof. M. Carmen Galan, University of Bristol, UK

Innovation in Organic Synthesis Prizewinners:

2004 Andrea Basso (University of Genova)

2005 Marco Lombardo (University of Bologna)

2006 Leonardo Manzoni (ISTM-CNR Milano)
& Ernesto Giovanni Occhiato (University of Firenze)

2007 Pier Giorgio Cozzi (University of Bologna)

2008 Gianluca Maria Farinola (University of Bari)

2009 Vito Capriati (University of Bari)

2010 Stefano Cicchi (University of Firenze)

2011 Maurizio Fagnoni (University of Pavia)

2012 Laura Cipolla (University of Milano-Bicocca)

2013 Cosimo Cardellicchio (CNR-ICCOM)

2014 Maurizio Benaglia (University of Milano)
& Renzo Luisi (University of Bari)

2015 Serena Perrone (University of Salento)

2016 Alessandro Abbotto (University of Milano-Bicocca)

2017 Raffaella Mancuso (University of Calabria)

2018 Oscar Francesconi (University of Firenze)

2019 Daniela Montesarchio (University of Napoli Federico II)

2020 Stefano Menichetti (University of Firenze)

2021 Marco Lombardo (University of Bologna)

2022 Sergio Rossi (University of Milano)

2023 Andrea Porcheddu (University of Cagliari)

2024 Alessandro Palmieri (University of Camerino)

Best PhD Thesis Prizewinners:

2003 Luigi Anastasia (University of Milano)

2004 Luca Bernardi (University of Bologna)

2005 Matilde Guala (University of Pavia)
& Carlo Punta (Politecnico di Milano

2006 Alberto Bossi (University of Milano)

2007 Stefano Protti (University of Pavia)

2008 Giacomo Ghini (University of Firenze)

2009 Anna Llanes-Pallas (University of Trieste)

2010 Patrizia Galzerano (University of Bologna)

2011 Elisa Mosconi (University of Bologna)

2012 Alex Manicardi (University of Parma)

2013 Nicola Castellucci (University of Bologna)

2014 Eleonora Tenori (University of Firenze)
& Michele Mingozzi (University of Milano)

2015 Massimo Manuelli (University of Firenze)

2016 Stefano Fedeli (University of Firenze)
& Vincenzo Campisciano (University of Palermo)

2017 Luka Đorđević (University of Trieste)

2018 Gianluca Salerno (University of Firenze)
& Claudia Riccardi (University of Napoli Federico II)

2019 Giulio Bertuzzi (University of Bologna)

2020 Marco Colella (University of Bari)

2021 Antonia Rinaldi (University of Firenze)

2022 Gianluca Casotti (University of Pisa)

2023 Enrico Marcantonio (University of Parma)

2024 Giulia Brufani (University of Perugia)

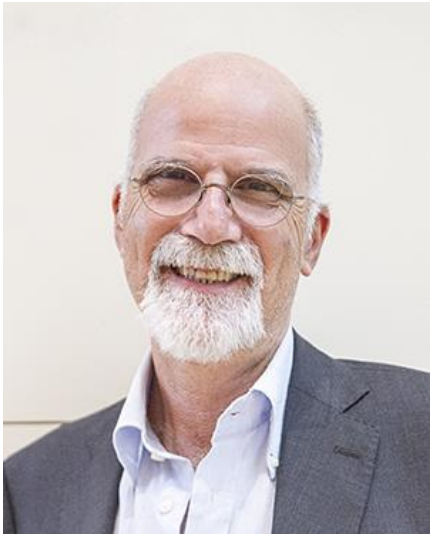
Plenary Speakers 2025:

Prof. M. Carmen Galan

University of Bristol, UK

CINMPIS Lecturer

Lecture: ***Controlling G4 DNA topology with small molecules: towards the development of novel therapeutics***



Prof. Maurizio Prato

CIC bioMagune,

San Sebastian, Spain

Lecture: ***Carbon nanodots: the missing link between the molecular and the nanoscale worlds***

Prizewinners 2024:

Innovation in Organic Synthesis 2024

Prof. Alessandro Palmieri

University of Camerino

Prize Lecture: ***Continuous flow synthesis and derivatization of homo- and heterocyclic systems***

Best PhD Thesis 2024

Dr. Giulia Brufani

University of Perugia

Prize Lecture: ***Sustainable synthetic methodologies for the synthesis of heterocyclic compounds***

Keynote Speakers 2025:

(in alphabetical order)

Prof. Luca Beverina (Università di Milano-Bicocca)

Prof. Sergio Mauricio Bonesi (University of Buenos Aires)

Prof. Giancarlo Cravotto (Università di Torino)

Prof. Leonardo Degennaro (Università di Bari Aldo Moro)

Prof. Carmine Gaeta (Università di Salerno)

Prof. Giuseppe Gattuso (Università di Messina)

Prof. Andrea Gualandi (Università di Bologna)

Prof. Loredana Maiuolo (Università della Calabria)

Prof. Enrico Marcantoni (Università di Camerino)

Prof. Domenica Musumeci (Università di Napoli Federico II)

Prof. Alessandra Operamolla (Università di Pisa)

Prof. Daniele Passarella (Università di Milano Statale)

Prof. Serena Riela (Università di Catania)

Prof. Giuseppe Sforazzini (Università di Cagliari)

Scientific programme:

	CINMPIS DAYS 2025
February 17, 2025	
8:00-9:00	**REGISTRATION**
9:00-9:25	***Opening Ceremony*** **prof. Angela Zampella,** *vice-Rector of University of Naples Federico II* **prof. Vito Capriati**, *Director of CINMPIS Consortium* **prof. Gianluca Farinola**, *President of the Italian Chemical Society (SCI)* **prof. Maria Valeria D'Auria**, *Past-President of the Organic Division of SCI* **prof. Daniela Montesarchio**, *Chair of CINMPIS Days 2025*
	Section 1: Chair prof. Daniela Montesarchio
9:25-10:05	**PL1 prof. M. Carmen Galan (*University of Bristol, UK*)** **CINMPIS LECTURER** Controlling G4 DNA topology with small molecules: towards the development of novel therapeutics
	Section 2: Chair prof. Marino Petrini
10:05-10:30	**KS1 prof. Enrico Marcantoni (*University of Camerino*)** The use of organic synthesis to tackle problems in chemical biology: climacostol and its analogues
10:30-10:55	**KS2 prof. Daniele Passarella (*University of Milano Statale*)** Natural products: exploring novel synthetic routes and chemical space
10:55-11:00	**FP1 dr. Anna Esposito (*University of Napoli Federico II*)** Mirror-image iminosugars: multipotent glycomimetics for the treatment of rare diseases
11:00-11:05	**FP2 dr. Giorgia Fracchioni (*University of Pavia*)** Exploring heptacyclic ligands: how oligo-heteroaryls interact with G-quadruplex motifs
11:05-11:35	**Coffee Break**
	Section 3: Chair prof. Maurizio Benaglia

11:35-12:00	**KS3 prof. Luca Beverina (*University of Milano Bicocca*)** Conjugated materials from and into interface rich, water based microheterogeneous environments
12:00-12:15	**OC1 prof. Erica Locatelli (*University of Bologna*)** Surface modification of nanocellulose towards additive manufacturing
12:15-12:30	**OC2 dr. Carola Ricciardelli (*University of Bari Aldo Moro*)** Disclosing the properties of silk fibroin in heterogeneous catalysis
12:30-12:45	**OC3 prof. Chiara Maria Antonietta Gangemi (*University of Messina*)** Lighting up tyrosinase inhibitors
12:45-13:00	**OC4 prof. Valentina Sepe (*University of Napoli Federico II*)** Discovery of new leukemia inhibitory factor receptor antagonists: 4,9-estradien-3-one scaffold
13:00-13:15	**OC5 dr. Emanuele Casali (*University of Pavia*)** The dual role of TEMPO in electrooxidative allene dioxygenation
13:15-13:30	**OC6 dr. Fabricio Nicolas Molinari (*University of Messina*)** Development of graphene-based solid sorbents for CO_2 capture
13:30-13:35	**FP3 dr. Giulia Romagnoli (*University of Siena*)** From micellar catalysed hydroformylation and hydroaminomethylation to solid waste-based sustainable processes
13:35-14:45	**Lunch Break**
	Section 4: Chair prof. Filippo Doria
14:45-15:10	**KS4 prof. Serena Riela (*University of Catania*)** Halloysite: unlocking the potential of a natural nanomaterial
15:10-15:35	**KS5 prof. Alessandra Operamolla (*University of Pisa*)** Lignin: a new and invaluable resource for organic devices
15:35-16:00	**KS6 prof. Domenica Musumeci (*University of Napoli Federico II*)** Focus on nucleoamino acids and nucleopeptides: from nucleic acid binding to self-assembling properties
16:00-16:15	**OC7 dr. Valentina Pirota (*University of Pavia*)** Fascinating ploy to the controlled orthogonalization of water-soluble naphthalene diimides
16:15-16:30	**OC8 prof. Andrea Calcaterra (*University of Roma La Sapienza*)** Studies towards the synthesis of vismione E
16:30-16:45	**OC9 dr. Mara Pulpito (*University of Bari Aldo Moro*)** One-pot two-step chemoenzymatic deracemization of secondary alcohols in iron-based deep eutectic solvents
16:45-17:15	**Coffee Break**
	Section 5: Chair prof. Stefano Superchi

17:15-17:40	**KS7 prof. Sergio Mauricio Bonesi (*University of Buenos Aires*)** Application of the photo-FRIES rearrangement reaction in organic synthesis
17:40-18:05	**KS8 prof. Giuseppe Sforazzini (*University of Cagliari*)** Light at work: molecular engineering of π-conjugated compounds towards responsive materials
18:05-18:20	**OC10 dr. Antonio Ricci (*Fresenius Kabi*)** Tackling operative challenges in the industrial pharmaceutical manufacturing processes framework
18:20-18:35	**OC11 dr. Gabriele Prina Cerai (*Procos*)** Process development and optimization: a case study on telescopic double Sonogashira reactions
	Section 6: Chair prof. Marco Bandini
18:35-18:40	**FP4 dr. Andrea Citarella (*University of Milano Statale*)** Synthesis of 1,2,3-triazoles in the green solvent cyrene
18:40-18:45	**FP5 dr. Marta Grazioli (*University of Pavia*)** Synthesis of herboxidiene derivatives as splicing modulators
18:45-18:50	**FP6 dr. Maria Grazia Nolli (*University of Napoli Federico II*)** Mild-temperature hydrosilylation for efficient functionalization of porous silicon biosensor for troponin detection during myocardial infarction
18:50-18:55	**FP7 dr. Gabriele Cianfoni (*University of Roma La Sapienza*)** Design and synthesis of polyamines to develop highly performing ferritin-conjugates
18:55-19:00	**FP8 dr. Fabiana Esposito (*University of Napoli Federico II*)** Semi-synthetic pathways to obtain glycosaminoglycans mimetics from sustainable sources
19:00-19:05	**FP9 dr. Margherita Miele (*University of Torino*)** Carbenoid-like strategies for expanding the chemical space of halogen-containing manifolds
19:05-19:10	**FP10 dr. Elisabetta Tomarchio (*University of Catania*)** Sustainable biopolymeric catalytic system for *suzuki-miyaura* reactions in aqueous media
19:10-19:15	**FP11 dr. Andrea Paparella (*University of Bari Aldo Moro*)** Embracing a new frontier: mastering Nickel-catalyzed cross-electrophile coupling reactions in deep eutectic solvents

19:15-19:20	**FP12 dr. Rita Mocci (*University of Cagliari*)** Mechanochemical synthesis of secondary amines via borrowing hydrogen strategy
19:20-19:25	**FP13 dr. Gianfranco Cavallaro (*University of Catania*)** In silico design of new antibacterial drugs and ligand-protein interaction studies targeting COX-1
19:25-19:30	**FP14 dr. Rossella Aronne (*University of Siena*)** Automatic computational protocol to explore G-quadruplex's binding sites through molecular dynamic simulations and virtual screening

20:30 Free Dinner

February 18, 2025	
	Section 7: Chair prof. Vito Capriati
9:00-9:45	**PL2 prof. Maurizio Prato (*CIC bioMagune, San Sebastian, Spain*)** Carbon nanodots: the missing link between the molecular and the nanoscale worlds
9:45-10:10	**KS9 prof. Alessandro Palmieri (*University of Camerino*)** **Prize: Innovation in Organic Synthesis 2024** Continuous flow synthesis and derivatization of homo- and heterocyclic systems
	Section 8: Chair prof. Walter Cabri
10:10-10:35	**KS10 prof. Andrea Gualandi (*University of Bologna*)** Developing Nickel organometallic nucleophilic reagents via photoredox catalysis
10:35-10:50	**OC12 dr. Patrizio Russo (*University of Calabria*)** Pd-Catalyzed coupling of 1-(2-(allyloxy)phenyl)-2-yn-1-ols and isonitriles for the synthesis of 2-(benzofuran-2-yl)acetamides
10:50-10:55	**FP15 dr. Giulio Bertuzzi (*University of Bologna*)** The gold-allene system for the functionalization of 7- and 4-membered rings
10:55-11:00	**FP16 dr. Giulia Monda (*University of Bologna*)** Direct access to benzalactams and benzolactones via Nickel-catalyzed carbonylation with CO_2
11:00-11:30	**Coffee Break**

	Section 9: Chair prof. Bartolo Gabriele
11:30-11:55	**KS11 prof. Giancarlo Cravotto (*University of Torino*)** New technologies and green protocols for industrial chemical process intensification
11:55-12:20	**KS12 prof. Leonardo Degennaro (*University of Bari Aldo Moro*)** Use of sustainable technologies enabling direct fluoroalkylation and fluorocarbonylation strategies
12:20-12:45	**KS13 prof. Loredana Maiuolo (*University of Calabria*)** 1,3-dipolar cycloaddition: a versatile method to synthesize small heterocycles and hybrid molecules
12:45-13:00	**OC13 prof. Alessandra Puglisi (*University of Milano Statale*)** Recycling of rare earth elements: from E-waste to stereoselective catalytic reactions
13:00-13:15	**OC14 dr. Fabio Pesciaioli (*University of L' Aquila*)** Expanding the boundaries of organocatalysis towards sustainability via acid and aminocatalysis
13:15-13:30	**OC15 dr. Chiara Zagni (*University of Catania*)** Hydroxypyrone-based materials: dual functionality for antimicrobial iron chelation and water pollutant degradation
13:30-14:45	**Lunch Break**
	Section 10: Chair prof. Alessandra Tolomelli
14:45-15:10	**KS14 prof. Giuseppe Gattuso (*University of Messina*)** Self-assembly of supramolecular polymers based on ionizable bis-pillar[5]arene monomers for sensing applications
15:10-15:35	**KS15 prof. Carmine Gaeta (*University of Salerno*)** Exploring prismarene: an emerging macrocyclic host in supramolecular chemistry
15.35-15.50	**OC16 prof. Sebastiano Di Pietro (*University of Pisa*)** Glycoconjugated luminescent lanthanide complexes as diagnostic probes
15:50-16:05	**OC17 dr. Serena Traboni (*University of Napoli Federico II*)** A new, straightforward synthesis of 3-deoxy-3-amino galactose, a key structural motif of galectin ligands
16:05-16:20	**OC18 dr. Federico Lami (*University of Milano Bicocca*)** Design and synthesis of a new Toll Like Receptor 4 agonist-based antibody drug conjugate for cancer immunotherapy
16:20-16:35	**OC19 dr. Ernesto Santoro (*University of Basilicata*)** Chiral molecular recognition by prism[n]arenes macrocycles

16:35-16:50	**OC20 dr. Alberto Luridiana (*University of Cagliari*)** A novel photocatalyzed strategy for the telescopic synthesis of substituted 1-pyrrolines
16:50-16:55	**FP17 dr. Ester Colarusso (*University of Salerno*)** Development of a one-pot, solvent-free reaction for the synthesis of fluoroquinolone antibiotic chemical core
16:55-17:00	**FP18 dr. Samuele Ruffoli (*University of Bologna*)** Study of the CISS effect through chiral peptide dyads
17:00-17:05	**FP19 dr. Maria Teresa Tiberi (*University of Perugia*)** Waste-minimized access to diarylamines and triarylamines via Csp^2–N coupling under batch and flow conditions
17:05-17:35	**Coffee Break**
	Section 11: Chair prof. Antonio Rescifina
17:35-18:00	**KS16 dr. Giulia Brufani (*University of Perugia*)** **Prize: Best PhD Thesis 2024** Sustainable synthetic methodologies for the synthesis of heterocyclic compounds
18:00-18:15	**OC21 prof. Marco Blangetti (*University of Torino*)** Oxidative anionic homo-Fries rearrangement under bench-type aerobic conditions
18:15-18:30	**OC22 dr. Alessio Petrellini (*University of Camerino*)** Fluorinated climacostol, a new potential small molecule cancer chemotherapeutic agent
18:30-18:45	**OC23 dr. Roberta Amuso (*University of Calabria*)** Sequential insertion of carbon monoxide and carbon dioxide for the synthesis of benzoxazinone derivatives
18:45-19:00	**OC24 dr. Alessandro Santarsiere (*University of Basilicata*)** Reactivity insights of arylboronic acids in *ipso*-substitution reactions
19:00-19:15	**OC25 dr. Stefano Barranco (*University of Cagliari*)** New synthetic methodologies for the chemo- and stereoselective transformation of substituted cyclobutanes
19:15	***Concluding Remarks & Greetings***

20:30 Social Dinner at Ristorante "La Bersagliera"

Plenary Lectures

PL n° 1

CONTROLLING G4 DNA TOPOLOGY WITH SMALL MOLECULES: TOWARDS THE DEVELOPMENT OF NOVEL THERAPEUTICS

M. Carmen Galan

School of Chemistry, University of Bristol, Cantock's Close, Bristol, United Kingdom

e-mail: m.c.galan@bristol.ac.uk

G-quadruplexes oligonucleotides (G4) are a fascinating class of nucleic acid structures formed from the self-association of guanine-rich sequences. This type of four-stranded structures have found potential applications in biological chemistry and responsive nanotechnology that may be exploited for therapeutic effect. While many examples of ligands that are able to stabilize G4 sequence are reported in the literature, those ligands do not induce reversible and controllable structural perturbations such as the re-folding of the G4 to an alternative topology or the unfolding of the G4 structure through binding modes at physiological pH. In this sense, light offers high spatiotemporal precision for the regulation of oligonucleotide structure and facilitates the investigation of how topological changes influence biological function.[1]
During this lecture I will describe recent examples of photoresponsive ligands for G4 DNA regulations developed within our research group. Examples of stiff-stilbene ligands which are capable of unfolding G4 DNA in physiological conditions in a reversible manner[2] to dithienylethene chromophores or novel diazobenzene molecules with inherently superior photoresponsive properties will be showcased.[3]

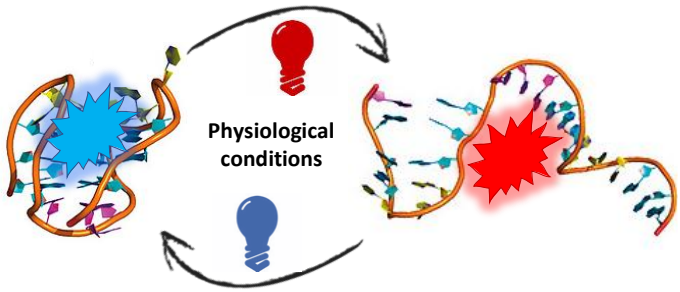


Figure 1.

[1] J. Ramos-Soriano and M. C. Galan, Photoresponsive control of G-Quadruplex DNA cystems *J. Am. Chem. Soc. Au* **2021**, *1*, 10, 1516.
[2] a) M. P. O'Hagan, S. Haldar, M. Duchi, T. A. A. Oliver, A. J. Mulholland, J. C. Moralres, M. C. Galan, A Photoresponsive stiff-stilbene ligand fuels the reversible unfolding of G-quadruplex DNA, *Angew. Chem. Int. Ed.*, **2019**, *58*, 4334-4338. b) M. P. O'Hagan, S. Haldar, J. C. Morales, A. J. Mulholland, M. C. Galan Enhanced sampling molecular dynamics simulations correctly predict the diverse activities of a series of stiff-stilbene G-quadruplex DNA ligands *Chem. Sci.* **2021**, *12*, 1415
[3] a) M. P. O'Hagan, J. Ramos-Soriano, S. Haldar, J. C. Moralres, A. J. Mulholland, M. C. Galan, Visible-light photocontrol of G-quadruplex ligand activity: toggling binding mode and oligonucleotide folding in physiological conditions *Chem. Commun.,* **2020**, *56*, 5186; b) J. Ramos-Soriano, Y.J. Jiang, B. Deng, M. O'Hagan, S. Haldar, A. Grao, S. OIiveira, A. Mulholland, M.C. Galan A bridged azobenzene derivative exhibits fully-reversible photocontrolled binding to a G-quadruplex DNA/duplex junction *ChemRxiv.* **2024**, doi:10.26434/chemrxiv-2024-7056b.

CINMPIS DAYS 2025, CINMPIS Lecturer

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2017-date	Professor in Organic and Biological Chemistry, University of Bristol
2015-2017	Reader in Organic and Biological Chemistry, University of Bristol
2013-2015	Senior Lecturer in Organic Chemistry, University of Bristol
2012-2017	EPSRC Career Acceleration Fellow, University of Bristol
2008-2012	Royal Society Dorothy Hodgkin Fellow, University of Bristol
2006-2008	Lecturer in Organic Chemistry, University of Bristol
2005-2006	Massachusetts Institute of Technology, Cambridge, USA, Post-Doctoral Fellow. Research Advisor: Prof. Sarah E. O'Connor
2003-2005	The Scripps Research Institute, La Jolla, CA, USA Post-Doctoral Research Associate. Research Advisor: Prof. C. H. Wong
1998-2002	Complex Carbohydrate Research Center, The University of Georgia, Athens, USA, Ph.D. in Organic Chemistry. Advisor: Prof. G.J. Boons

Research Interests:
Organic and biological chemistry, G-quadruplexes, carbohydrate chemistry, functional nanomaterials.

Selected Publications:

1. M. Pérez-Soto, J. Ramos-Soriano, P. Peñalver, E. Belmonte-Reche, M. P. O'Hagan, J.-L. Mergny, M. C. Galan, M. C. Lopez-Lopez, M. C. Thomas, J.C. Morales, DNA G-quadruplexes in the genome of trypanosoma cruzi as potential therapeutic targets for chagas disease: dithienylethene ligands as effective antiparasitic agents. *Eur. J. Med. Chem*. **2024**, *276*, 116641
2. J. Ramos-Soriano, Y.J. Jiang, B. Deng, M. O'Hagan, S. Haldar, A. Grao, S. OIiveira, A. Mulholland, M.C. Galan, A bridged azobenzene derivative exhibits fully-reversible photocontrolled binding to a G-quadruplex DNA/duplex junction. *ChemRxiv*. **2024**; doi:10.26434/chemrxiv-2024-7056b
3. J. Ramos-Soriano, M. Holbrow-Wilshaw, E. Hunt, Y.J. Jiang, P. Peñalver, J.C. Morales, M.C. Galan, Probing the binding and antiparasitic efficacy of azobenzene G-quadruplex ligands to investigate G4 ligand design. *Chem Commun.* **2024**, *60*, 11520-11523.
4. M. P. O'Hagan, S. Haldar, J. C. Morales, A. J. Mulholland, M. C. Galan, Enhanced sampling molecular dynamics simulations correctly predict the diverse activities of a series of stiff-stilbene G-quadruplex DNA ligands. *Chem. Sci.* **2021**, *12*, 1415.
5. S. T. G. Street, P. Peñalver, M. P. O'Hagan, G.J. Hollingworth, J. C. Morales, M. C. Galan, Imide condensation as a strategy for the Synthesis of core diversified G-quadruplex ligands with anticancer and anti-parasitic activity. *Chem. Eur. J.* **2021**, *27*, 1.
6. M. O'Hagan, J. Ramos Soriano, S. Haldar, S. Sheik, A. J. Mulholland, J.C. Morales, M. Carmen Galan, Visible-light photoswitching of ligand binding mode suggests G-quadruplex DNA as a target for photopharmacology. *Chem. Commun.* **2020**, *56*, 5186.
7. M.P. O'Hagan, S. Haldar, M. Duchi, T.A.A. Oliver, A. J. Mulholland, J.C. Morales, M.C. Galan, A photoresponsive stiff-stilbene ligand fuels the reversible unfolding of G-quadruplex DNA. *Angew. Chem. Int. Ed.* **2019**, *131*, 1.

PL n° 2

CARBON NANODOTS: THE MISSING LINK BETWEEN THE MOLECULAR AND THE NANOSCALE WORLDS

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In recent years, the focus of nanoscience and nanotechnology has gradually shifted from the synthesis of individual components to their assembly into larger systems and materials. Indeed, the precise organization of matter across multiple length scales is of particular interest because of its great potential for advanced functions and properties.
We have recently described a simple, scalable, reliable and cost-effective synthetic process for producing high-quality carbon nanodots (CNDs), employing arginine and ethylenediamine as precursors [1,2]. The new material displays small size and high fluorescence quantum yields. Moreover, CNDs can be easily post-functionalized, due to the abundant presence of amino groups.
We have also presented a rational synthetic design for mastering CND properties, showing the importance in the choice of the precursors. By using properly designed functional units, the desired properties can be modulated, from the molecular to the nanoscale level in a controlled fashion. CNDs with customized emission can therefore be approached. Green and white-emitting CNDs were synthesized [3,4]. Also, the electrochemical properties of suitably synthesized CNDs can be modulated, while chiral CNDs can be prepared starting from chirally stable substrates [4,5]. Finally, the CNDs can be proficiently used in organocatalysis, or even in stereoselective syntheses.
During this talk, we will communicate our latest results in this fast-developing field.

Financial support from the European Research Council (ERC ADG-2019, grant nº 885323, is gratefully acknowledged.

[1] L. Dordevic, F. Arcudi, M. Cacioppo, M. Prato, *Nat. Nanotechnol.* **2022**, *17*, 112.
[2] F. Arcudi, L. Dordevic, M. Prato, *Angew. Chem. Int. Ed.* **2016**, *55*, 2107.
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[4] L. Dorđevic, F. Arcudi, A. D'Urso, M. Cacioppo, N. Micali, T. Bürgi, R. Purrello, M. Prato, *Nat. Commun.* **2018**, *9*, 3442.
[5] B. Bartolomei, V. Corti, M. Prato, *Angew. Chem. Int. Ed.* **2023**, *62*, e202305460.

CINMPIS DAYS 2025, Plenary Lecture n. 2

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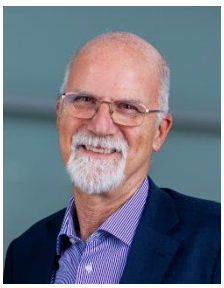

2015–Present	Ikerbasque Research Professor, CIC biomaGUNE, San Sebastián, Spain
2000–2023	Full Professor, University of Trieste, Italy
1992–2000	Associate Professor, University of Trieste, Italy
1983–1992	Assistant Professor, University of Padova, Italy
1986–1987	Visiting researcher, Yale University, USA
1991–1992	Visiting scientist, University of California, Santa Barbara, USA

Research Interests:

Materials science, nanomedicine, spinal cord repair, production of hydrogen from water.

Selected Publications:

1. B. Bartolomei, M. Sbacchi, C. Rosso, A. Günay-Gürer, L. Zdrazil, A. Cadranel, S. Kralj, D.M. Guldi, M. Prato, Synthetic strategies for the selective functionalization of carbon nanodots allow optically communicating suprastructures, *Angew. Chem. Int. Ed.*, **2024**, *63,* e202316915.
2. B. Bartolomei, V. Corti, M. Prato, Chiral carbon nanodots can act as molecular catalysts in chemical and photochemical reactions, *Angew. Chem. Int. Ed.*, **2023**, *62,* e202305460.
3. T. Gobbato, F. Rigodanza, E. Benazzi, P. Costa, M. Garrido, A. Sartorel, M. Prato, M. Bonchio, Enhancing oxygenic photosynthesis by cross-linked perylenebisimide "Quantasomes", *JACS*, **2022**, *144*, 14021-14025.
4. J. Dosso, B. Bartolomei, N. Demitri, F.P. Cossío, M. Prato, Phenanthrene-extended phenazine dication: an electrochromic conformational switch presenting dual reactivity, JACS, **2022**, *144*, 7295-7301.
5. L. Dordevic, F. Arcudi, M. Cacioppo, M. Prato, A multifunctional chemical toolbox to engineer carbon dots for biomedical and energy applications, *Nature Nanotechnology* **2022**, *17*, 112–130.
6. M. Bonchio, Z. Syrgiannis, M. Burian, N. Marino, E. Pizzolato, K. Dirian, F. Rigodanza, G. A. Volpato, G. La Ganga, N. Demitri, S. Berardi, H. Amenitsch, D. M. Guldi, S. Caramori, C. A. Bignozzi, A. Sartorel, M. Prato, Hierarchical organization of perylene bisimides and polyoxometalates for photo-assisted water oxidation, *Nature Chemistry* **2019**, *11*, 146–153.
7. N.P. Pampaloni, M. Lottner, M. Giugliano, A. Matruglio, F. D'Amico, M. Prato, J.A. Garrido, L. Ballerini, D. Scaini, Single-layer graphene modulates neuronal communication and augments membrane ion currents *Nature Nanotechnology*, **2018**, *13*, 755-764.

Keynote Lectures

KS n° 1

THE USE OF ORGANIC SYNTHESIS TO TACKLE PROBLEMS IN CHEMICAL BIOLOGY: CLIMACOSTOL AND ITS ANALOGUES

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Chemical biology highlights every day the fundamental role of organic synthesis in providing that multidisciplinary approach through which scientists, working at the interface of organic chemistry and biology, can aim to develop the most effective therapeutic agents against major diseases [1]. Even if immunotherapeutic and other macromolecules have become more prominent in the chemotherapy landscape, small molecules still have important advantages. The lower manufacturing costs, pharmacokinetic versatility, simplicity of storage and transportation, and other practical benefits of small molecules cement their place in disease treatment [2]. We have been studying for several years small molecules such as climacostol (**1**) and its analogues (**2-6**), and the synthetic results obtained provide useful contributions to chemical biology capable of opening new paths for a better life [3-5]. By minimizing unpleasant or harmful side effects, in particular, these small molecules can increase patient compliance, which leads to better treatment success.

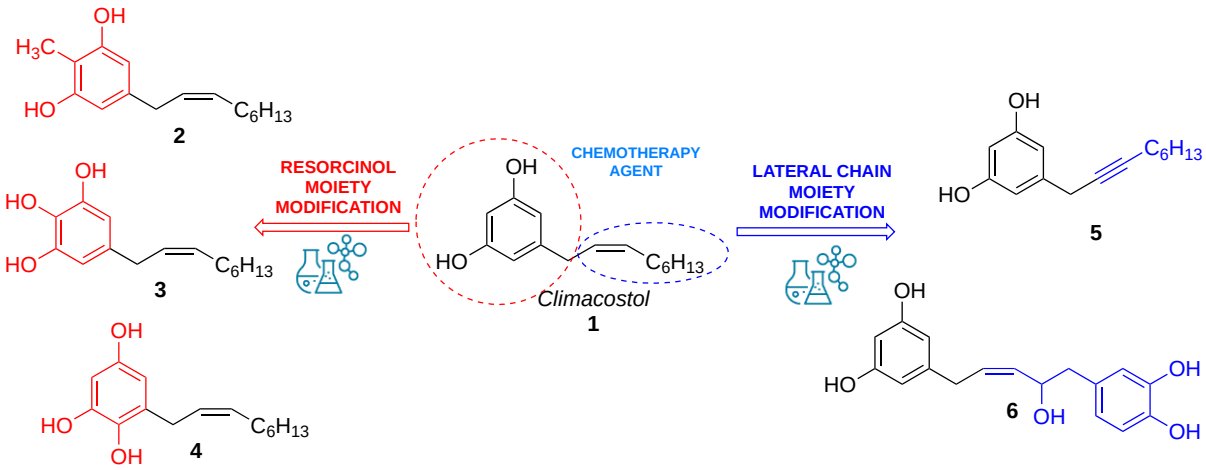

Figure 1.

[1] V. Percec, Q. Xiao, *Giant* **2020**, *4*, 100036.
[2] K. H. Nam, *Int. J. Mol. Sci.* **2021**, *22*, 3761.
[3] F. Buonanno, E. Catalani, D. Cervia, C. Cimarelli, E. Marcantoni, C. Ortenzi, *Microorganism* **2020**, *8*, 809.
[4] E. Catalani, F. Buonanno, G. Lupidi, S. Bongiorni, R. Belardi, S. Zecchini, M. Giovarelli, Marco Coazzoli. C. De Palma, C. Perrotta, E. Clementi, G. Prantera, E. Marcantoni, C. Ortenzi, A. M. Fausto, S. Picchietti, D. Cervia, *Front. Chem.* **2019**, *7*, 463.
[5] F. Buonanno, E. Catalani, D. Cervia, F. P. Serafini, S. Picchietti, A. M. Fausto, S. Giorgi, G. Lupidi, F.V. Rossi, E. Marcantoni, D. Petrelli, C. Ortenzi, *Toxins* **2019**, *11*, 42.

CINMPIS DAYS 2025, Keynote Lecture n. 1

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2005–Present	Full Professor, University of Camerino, Italy
2000–2004	Associate Professor, University of Camerino, Italy
1990–1999	Assistant Professor, University of Camerino, Italy
1994–1995	Visiting researcher, Colorado State University, Fort Collins, USA
1987 MA	University of Camerino, Italy

Research Interests:
Catalytic reactions, natural products, synthesis biology, sustainable organics.

Selected Publications:

1. G. Lupidi, E. Catalani, F. Buonanno, D. Gentili, S. Giorgi, V.A.Vishnuprasad Ponnarassery, S. Gabrielli, K. Brunetti, A.M. Fausto, S. Picchietti, C. Ortenzi, E. Marcantoni, D. Cervia, Chemical modification for improving drug-like molecular properties of climacostol, a natural resorcinolic lipid, *Bioorg. Med. Chem.* **2025**, *119*, under review.
2. D. Gentili, E. Marcantoni, M. Tiecco, A. Palmieri, Investigations on the use of Deep Eutectic Solvents (DESs) as promoters for the conjugate addition of α-nitro ketones to electron-poor alkenes, *ChemistrySelect* **2024**, *9*, e202401251.
3. G. Pastore, S. Gabrielli, R. Giacomantonio, G. Lupidi, S. Capodaglio, F. Stella, E. Leone, T. Compagnucci, E. Marcantoni, An efficient synthesis of bio-based poly(urethane-acrylate) by SiO_2-supported $CeCl_3.7H_2O$-NaI as recyclable catalyst. *Results in Materials* **2022**, *15*, 100294.
4. F.V. Rossi, D. Gentili, E. Marcantoni, Metal-promoted heterocyclization: a heterosynthetic approach to face a pandemic crisis. *Molecules* **2021**, *26*, 2620.
5. S. Zecchini, F. Proietti Serafini, E. Catalani, M. Giovarelli, M. Cazzoli, I. Di Renzo, C. De Palma, C. Perrotta, E. Clementi, F. Buonanno, C. Ortenzi, E. Marcantoni, A.R. Taddei, S. Picchietti, A.M. Fausto, D. Cervia, Dysfunctional autophagy induced by the pro-apoptotic natural compound climacostol in tumor cells. *Cell Death Dis.* **2019**, *10*, 10.
6. F. Buonanno, E. Catalani, D. Cervia, F. Proietti Serafini, S. Picchietti, A.M. Fausto, S. Giorgi, G. Lupidi, F.V. Rossi, E. Marcantoni, D. Petrelli, C. Ortenzi, Bioactivity and structural properties of novel synthetic analogues of the protozoan toxin climacostol. *Toxins* **2019**, *11*, 42.
7. E. Marcantoni, A. Palmieri, M. Petrini, Recent synthetic applications of α-amido sulfones as precursors of N-acylimino derivatives. *Org. Chem. Front.* **2019**, *6*, 2142-2182.
8. E. Catalani, D. Proietti Serafini, Zecchini, S. Picchietti, A.M. Fausto, E. Marcantoni, F. Buonanno, C. Ortenzi, C. Perrotta, D. Cervia, Natural products from aquatic eukaryotic microorganism for cancer therapy: perspectives on anti-tumour properties of ciliate bioactive molecules. *Pharmacological Research* **2016**, *113*, 409-420.

KS n° 2

NATURAL PRODUCTS: EXPLORING NOVEL SYNTHETIC ROUTES AND CHEMICAL SPACE

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Natural products, particularly those with relevant pharmacological activities, have a long history. Their importance as an irreplaceable source in drug discovery and their unique behavior make them challenging targets in chemical synthesis. In our lab, we study natural products as key players in various research projects, fulfilling three different roles. We consider them as important target for the study of new total synthesis [1-3], as lead compounds for the rational design and synthesis of new analogs with new biological activities [4-5] and as building blocks for the construction of conjugate compounds with new properties [6]. The presentation will regard the representative cases belonging to three class of compounds: epothilones, cannabinoids, and glycybridins.

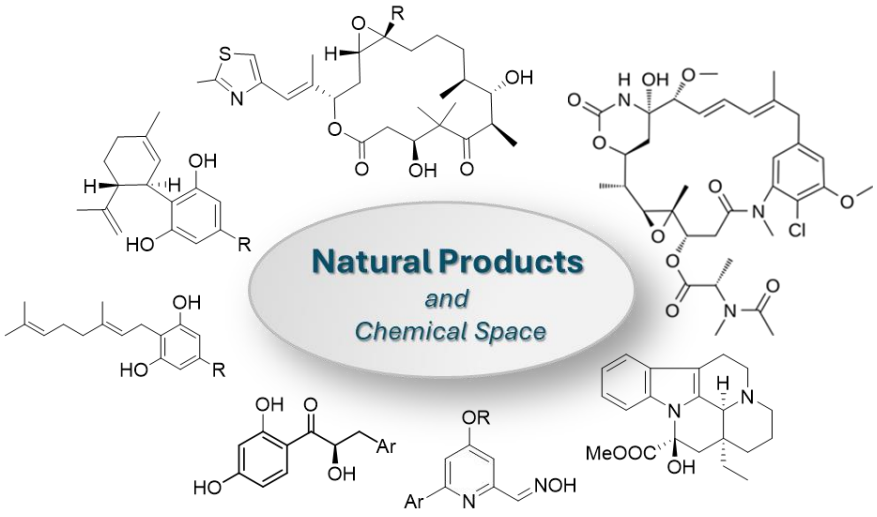

Figure 1.

[1] P. Marzullo. D. Passarella *et al.* Total synthesis of (-)-Cannabidiol-C4 *Eur. J. Org. Chem.* **2022**, e202200392
[2] A. Dimasi, V. Fasano, *et al. RSC Advances* **2024**, *14*, 5542–5546.
[3] A. Maiocchi, D. Passarella *et al.* Minor cannabinoids as inhibitors of skin inflammation: chemical synthesis and biological evaluation *J. Nat. Prod*. **2024**, *87*, 1725-1734.
[4] E. Colombo, D. Passarella *et al.* Total synthesis of an epothilone analogue based on the amide-triazole bioisosterism *ChemPlusChem*, **2024**, *89*, e202400413.
[5] E. Bonandi, D. Passarella, Design and synthesis of new withaferin a inspired hedgehog pathway inhibitors *Chem. Eur. J.* **2021**, *27*, 8350–8357.
[6] Z. Boiarska, D. Passarella, *et al.* Maytansinol functionalization: towards useful probes for studying microtubule dynamics *Chem. Eur. J.* **2023**, *29*, e202203431.

CINMPIS DAYS 2025, Keynote Lecture n. 2

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2020–Present	Full Professor, Università degli Studi di Milano, Italy
2006–2020	Associate Professor, Università degli Studi di Milano, Italy
1993–2006	Assistant Professor, Università degli Studi di Milano, Italy
1992	PostDoc, Universitad de Barcelona, Spain
1992 PhD	Università degli Studi di Milano, Italy

Research Interests:

Total synthesis, modification of natural products, preparation of quality collections of heterocyclic and natural compounds with biological interest, self-assembled nanoparticles, rationally design of proteolysis targeting chimeras.

Selected Publications:

1. E. Colombo, D. Coppini, S. Borsoi, V. Fasano, R, Bucci, F. Bonato, E. Bonandi, F. Vasile, S. Pieraccini, D. Passarella, Total synthesis of an epothilone analogue based on the amide ‑ triazole bioisosterism *ChemPlusChem.* **2024**, *89,* e202400413.
2. A. Maiocchi, M. Fumagalli, M. Vismara, A. Blanco, U. Ciriello, G. Paladino, S. Piazza, G. Martinelli, V. Fasano, M. Dell'Agli, D. Passarella, Minor Cannabinoids as inhibitors of skin inflammation: chemical synthesis and biological evaluation *J. Nat. Prod.* **2024**, *87*, 1725-1734.
3. Z. Boiarska, H. Pérez-Peña, A.C. Abel, P. Marzullo, Álvarez-Bernad, F. Bonato, B. Santini, D. Horvath, D. Lucena-Agell, F. Vasile, M. Sironi, J.F. Diaz, A. Prota, S. Pieraccini, D. Passarella, Maytansinol functionalization: towards useful probes for studying microtubule dynamics *Chem. Eur. J.* **2023**, *29*, e202203431.
4. E. Colombo, D. Coppini, S. Maculan, P. Seneci, B. Santini, F. Testa, L. Salvioni, G.-M.Vanacore, M. Colombo, D. Passarella, Folic acid functionalization for targeting self-assembled paclitaxel-based nanoparticles *RSC Advances* **2022**, *12*, 35484-35493.
5. P. Marzullo, A. Maiocchi, L. Lo Presti, U. Ciriello, G. Paladino, D. Passarella Total synthesis of (-)-cannabidiol-C4 *Eur. J. Org. Chem.* **2022**, e202200392.
6. P. Marzullo, Z. Boiarska, H. Pérez-Peña, A.C. Abel, B. Álvarez-Bernad, L. Lucena-Agell, F. Vasile, M. Sironi, K.-H. Altmann, A. Prota, J.-F. Diaz, S. Pieraccini, D. Passarella, Maytansinol derivatives: side reactions as a chance for new tubulin binders *Chem. Eur. J.* **2022**, 28, e20210352.
7. E. Bonandi, M. Mori, P. Infante, I. Basili, L. Di Marcotullio, A. Calcaterra, F. Catti, B. Botta, D. Passarella, Design and synthesis of new withaferin a inspired hedgehog pathway inhibitors *Chem. Eur. J.* **2021**, *27*, 8350–8357.

KS n° 3

CONJUGATED MATERIALS FROM AND INTO INTERFACE RICH, WATER BASED MICROHETEROGENEOUS ENVIRONMENTS

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Conjugated materials are key components for organic devices. Established materials were originally designed and developed with performances in mind and with rigorous exclusion of water from the environment they were supposed to work in. This scenario is rapidly changing according to both the drive for the substitution of organic solvents with water in synthesis and processing and with the ever-increasing number of applications requiring a water/organics interface. The general rule for organic conjugated compounds is that solubility in water is very poor, unless complex and invasive functionalization is performed.
Formulation chemists developed efficient strategies to homogeneously disperse and stabilize hydrophobic derivatives in water by means of suitable amphiphilic molecules possessing a hydrophilic and a hydrophobic domain, called surfactants. They are capable of sizably reducing the interfacial energy associated with the presence of hydrophobic derivatives in an aqueous environment. Above a certain concentration, most surfactants self-assemble in a variety of association colloids the most common of whom is the spherical micelle. At higher concentration, depending on the temperature and/or the ionic strength of the water solutions, more complex structures the like of microemulsions, lamellae, vesicles and tubules can also be observed.[1] The common characteristic of all such micro heterogeneous environments is the formation of lipophilic pockets within a polar environment where either additional surfactant or other lipophiles can be accommoPresentd. In the early ‘80s synthetic chemists started realizing that association colloids are a simplified analogous of enzymes: reagents can be hosted and selectively localized in an environment with specific polarity, possibly leading to improved yield and selectivity.[2,3] The talk will focus on the opportunities that the formulation chemistry toolbox offers for the green synthesis and processing of established and new materials that could not be made otherwise.[4] Association colloids also offers the possibility to colocalize in a confined environment of controlled polarity, mixtures of different compounds that can be engaged in complex photophysical processes of interests for biological imaging and more.[5]

[1] M. Sassi, S. Mattiello, L. Beverina, Eur. *J. Org. Chem.* **2020**, *26*, 3942–3953.
[2] M. Cortes-Clerget, N. Akporji, J. Zhou, F. Gao, P. Guo, M. Parmentier, F. Gallou, J.Y. Berthon, B.-H. Lipshutz, *Nature Comm.* **2019**, 1–10.
[3] C. Ceriani, E. Ghiglietti, M. Sassi, S. Mattiello, L. Beverina, *Org. Process Res. Dev.* **2020**.
[4] A. Sanzone, A. Calascibetta, M. Monti, S. Mattiello, M. Sassi, F. Corsini, G. Griffini, M. Sommer, L. Beverina, *ACS Macro Lett.* **2020**, *9* (8), 1167–1171.
[5] S. Mattiello, A. Monguzzi, J. Pedrini, M. Sassi, C. Villa, Y. Torrente, R. Marotta, F. Meinardi, L. Beverina, *Adv. Funct. Mater.* **2016**, *26* (46), 8447–8454.

CINMPIS DAYS 2025, Keynote Lecture n. 3

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2020–Present	Full Professor, University of Milano-Bicocca, Italy
2014–2019	Associate Professor, University of Milano-Bicocca, Italy
2005–2014	Assistant Professor, University of Milano-Bicocca, Italy
2004–2005	Visiting researcher, Georgia Institute of Technology, Atlanta (GA), USA
2003 PhD	University of Milano-Bicocca, Italy

Research Interests:
Organic (opto)electronics, (bio)photonics, green chemistry, catalysis, hybrid nanomaterials, formulation chemistry.

Selected Publications:

1. A. Zucchi, S. Mattiello, M. Sassi, L. Beverina, Straightforward, sustainable, and scalable access to 3,4-perylenedicarboxylic monoanhydride. *ACS Sustainable Chem. Eng.* **2024**, *12* (22), 8533–8540. https://doi.org/10.1021/acssuschemeng.4c02041.
2. S. Mattiello, A. Danos, K. Stavrou, A. Ronchi, R. Baranovski, D. Florenzano, F. Meinardi, L. Beverina, A. Monkman, A. Monguzzi, Diffusion-free intramolecular triplet-triplet annihilation contributes to the enhanced exciton utilization in OLEDs. *Adv. Opt. Mater.* **2024**, *12*, 2401597. https://doi.org/10.1002/adom.202401597.
3. F. Pallini, S. Mattiello, N. Manfredi, S. Mecca, A. Fedorov, M. Sassi, K. Al Kurdi, Y.-F. Ding, C.-K. Pan, J. Pei, S. Barlow, S.R. Marder, T.-Q. Nguyen, L. Beverina, Direct detection of molecular hydrogen upon p- and n-doping of organic semiconductors with complex oxidants or reductants. *J. Mater. Chem. A* **2023**, *11* (15), 8192–8201. https://doi.org/10.1039/D3TA00231D.
4. S. Mecca, F. Pallini, V. Pinchetti, A. Erroi, A. Fappani, F. Rossi, S. Mattiello, G.M. Vanacore, S. Brovelli, L. Beverina, Multigram-scale synthesis of luminescent cesium lead halide perovskite nanobricks for plastic scintillators. *ACS Appl. Nano Mater.* **2023**, acsanm.3c01146. https://doi.org/10.1021/acsanm.3c01146.
5. S. Mattiello, E. Ghiglietti, A. Zucchi, L. Beverina, Selectivity in micellar catalysed reactions. The role of interfacial dipole, compartmentalisation, and specific interactions with the surfactants. *Current Opinion in Colloid & Interface Science* **2023**, 101681. https://doi.org/10.1016/j.cocis.2023.101681.
6. C. Ceriani, M. Scagliotti, T. Losi, A. Luzio, S. Mattiello, M. Sassi, N. Pianta, M. Rapisarda, L. Mariucci, M. Caironi, L. Beverina, Organic solvent free synthesis and processing of semiconducting polymers for field effect transistors in waterborne dispersions. *Adv Elect Materials* **2023**, 2201160. https://doi.org/10.1002/aelm.202201160.
7. S. Mattiello, S. Mecca, A. Ronchi, A. Calascibetta, G. Mattioli, F. Pallini, F. Meinardi, L. Beverina, A. Monguzzi, Diffusion-free intramolecular triplet–triplet annihilation in engineered conjugated chromophores for sensitized photon upconversion. *ACS Energy Lett.* **2022**, 2435–2442. https://doi.org/10.1021/acsenergylett.2c01224.

KS n° 4

HALLOYSITE: UNLOCKING THE POTENTIAL OF A NATURAL NANOMATERIAL

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Halloysite nanotubes (HNTs), a naturally abundant and low-cost nanomaterial, have garnered significant interest due to their unique tubular structure, biocompatibility, and versatility. [1] The covalent grafting of functional groups onto their surface enhances their chemical reactivity, unlocking opportunities for applications such as encapsulation, controlled release, and catalysis. [2] Leveraging covalent chemistry, HNTs can act as a versatile platform for addressing pressing challenges in biomedicine, environmental science, and materials engineering. Herein, I will present key examples of how covalent modifications have enabled innovative solutions, including advanced drug delivery systems, stimuli-responsive nanocomposites, and eco-friendly adsorbents for pollutant removal.[3]

Figure 1.

ACKNOWLEDGEMENTS: "SiciliAn MicronanOTecH Research And Innovation CEnter "SAMOTHRACE" (MUR, PNRR-M4C2, ECS_00000022), spoke 3 - Università degli Studi di Palermo "S2-COMMs - Micro and Nanotechnologies for Smart & Sustainable Communities", spoke 1, WP2-Environment, Task “Application of new materials for the real-time control of contaminants of emerging concern in water”, PRIN 2022 PNRR “P2022YJZ5FPE5 and Linea di Intervento 1 - Progetti di Ricerca Collaborativa del “PIAno di inCEntivi per la RIcerca di Ateneo 2024/2026 -UniCt.

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CINMPIS DAYS 2025, Keynote Lecture n. 4

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2023–Present	Full Professor, University of Catania, Italy
2018–2022	Associate Professor, University of Palermo, Italy
2002–2017	Assistant Professor, University of Palermo, Italy
2018	Visiting researcher, University of Miami, USA
2019	Visiting researcher, University of Granada, Spain
2000 PhD	University of Bologna, Italy
1999-2000	Visiting PhD-student University California of Los Angeles, Los Angeles, USA

Research Interests:
Clay minerals, surface modifications, supramolecular chemistry, drug delivery systems.

Selected Publications:

1. P. Poma, M. Massaro, S. Rigogliuso, L. Condorelli, R. Sánchez-Espejo, C. Viseras-Iborra, M. Notarbartolo, S. Riela, Curcumin and doxorubicin encapsulated in biocompatible clay-based nanomaterial: a strategy to overcome multidrug resistance *ArchPharm* **2025**, *358*, 2400702.
2. A.P. Falanga, M. Massaro, M. Notarbartolo, G. Piccialli, L.F. Liotta, R. Sánchez-Espejo, C. Viseras-Iborra, F.M. Raymo, G. Oliviero, S. Riela, Carrier capability of halloysite nanotubes for the intracellular delivery of antisense PNA targeting mRNA of neuroglobin gene *J. Coll. Int. Sci* **2024**, *663*, 9-20.
3. G. Cinà, M. Massaro, G. Cavallaro, G. Lazzara, R. Sánchez-Espejo, C. Viseras-Iborra, B. D'Abrosca, A. Fiorentino, G.M.L. Messina, S. Riela, Development of alginate film filled with halloysite-carbon dots for active food packaging *Int. J. Biol. Macromol.* **2024**, *277*, 134375.
4. M. Massaro, M.L. Alfieri, G. Rizzo, F. Babudri, R. de Melo Barbosa, T. Faddetta, G. Gallo, A. Napolitano, R. Sánchez-Espejo, C. Viseras-Iborra, S. Riela, Modification of halloysite lumen with dopamine derivatives as filler for antibiofilm coating *J. Coll. Int. Sci* **2023**, *646*, 910-921.
5. M. Massaro, E. Licandro, S. Cauteruccio, G. Lazzara, L.F. Liotta, M. Notarbartolo, F.M. Raymo, R. Sánchez-Espejo, C. Viseras-Iborra, S. Riela, Nanocarrier based on halloysite and fluorescent probe for intracellular delivery of peptide nucleic acids *J. Coll. Int. Sci* **2022**, *620*, 221-233.
6. M.L. Alfieri, M. Massaro, M. d'Ischia, G. D'Errico, N. Gallucci, M. Gruttadauria, M. Licciardi, L.F. Liotta, G. Nicotra, G. Sfuncia, S. Riela, Site-specific halloysite functionalization by polydopamine: a new synthetic route for potential near infrared-activated delivery system *J. Coll. Int. Sci* **2022**, *606*, 1779-1791.
7. M. Massaro, M. Notarbartolo, F.M. Raymo, G. Cavallaro, G. Lazzara, M.M.A. Mazza, C. Viseras-Iborra, S. Riela, Supramolecular association of halochromic switches and halloysite nanotubes in fluorescent nanoprobes for tumor detection *ACS Appl. Nano Mater.* **2022**, *5*, 13729-13736.

KS n° 5

LIGNIN: A NEW AND INVALUABLE RESOURCE FOR ORGANIC DEVICES

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In recent decades, the urgent challenge of identifying effective alternatives to materials with uneven global distribution has garnered significant attention. Within the framework of a circular economy, lignocellulosic biomass has emerged as a plentiful and valuable resource for biopolymers, offering exciting potential in materials science. In this context, lignin, the second most abundant organic polymer in lignocellulosic biomass, has become a focus of growing interest.[1] Lignin is a polymer rich in aromatic rings, isolated as a byproduct of industrial cellulose production. However, recent research highlights the need to fully harness lignin's potential, including its application in sustainable batteries.[2]

Our recent studies have demonstrated that waste lignin derived from kraft pulping can serve as a dielectric layer in organic field-effect transistors.[3] Our ongoing investigations aim to further clarify the structural characteristics and properties of lignin extracted directly from raw biomass using the organosolv method.[4] These efforts also seek to expand lignin's applications to memory storage devices, paving the way for its broader use in advanced technologies.[5]

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[5] S. De Stefano, O. Durante, R. D'Orsi, A. Operamolla, M. Ambrico, P. F. Ambrico, N. Martuccello, F. Giubileo, A. Di Bartolomeo, Resistive switching memory from dielectric lignin for sustainable electronics, *Journal of Materials Chemistry C.* **2024**, *12*, 13621.

CINMPIS DAYS 2025, Keynote Lecture n. 5

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2010–2015 Post-Doctoral Fellow, Aldo Moro University of Bari, Italy
2010 Post-Doctoral Fellow, Johannes Kepler University, Linz, Austria
2009 PhD in Chemistry of Innovative Materials, Aldo Moro University of Bari, Italy

Research Interests:

Organic chemistry, natural compounds, biopolymers, materials science.

Selected Publications:

1. S.K. Ghosh, F. Matino, F. Lineu Favrin, I. Tonazzini, R. D'Orsi, J.G. de la Ossa, A. Camposeo, J. Li, W. Liu, T.A. Hacker, D. Pisignano, A. Operamolla, X. Wang, L. Persano, Fully-biodegradable hierarchically designed high-performance nanocellulose piezo-arrays, *Sci. Adv.* **2025**, *11*, eads0778.
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3. R. D'Orsi, N. Di Fidio, C. Antonetti, A.M. Raspolli Galletti, A. Operamolla, Isolation of pure lignin and highly digestible cellulose from defatted and steam-exploded cynara cardunculus, *ACS Sust. Chem. Eng.* **2023**, *11*, 1875–1887.
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5. L. Spagnuolo, R. D'Orsi, A. Operamolla, Nanocellulose for paper and textile coating: the importance of surface chemistry, *ChemPlusChem* **2022**, *87*(8), e202200204.
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KS n° 6

FOCUS ON NUCLEOAMINO ACIDS AND NUCLEOPEPTIDES: FROM NUCLEIC ACID BINDING TO SELF-ASSEMBLING PROPERTIES

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Nucleobase-containing amino acids (nucleoamino acids) and nucleobase-containing peptides (nucleopeptides, Fig. 1) show many interesting properties for various biomedical applications, including nucleic acid-binding ability, chelation to biologically relevant metal ions, or formation of supramolecular networks [1-3].
In the last two decades, we have explored several nucleoamino acids and nucleopeptides made of different nucleoamino acid monomers finding in various cases interesting properties in terms of binding to specific biomolecular targets, and of self-assembly [1-5].

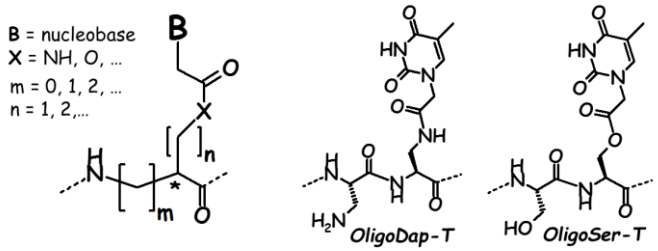

Figure 1. Generic nucleopeptide structure composed of a (α-, β-, γ-, etc.)peptide backbone on which nucleobases are anchored through suitable linkers, and two examples of nucleopeptides based on L-diaminopropanoic acid and L-serine backbones

Here, the chemical synthesis and characterization of some selected examples of nucleoamino acids/nucleopeptides, together with the investigation of their nucleic acid recognition ability, as well as self-assembling properties, will be presented.

[1] D. Musumeci, V. Roviello, G. N. Roviello, DNA- and RNA-binding ability of oligoDapT, a nucleobase-decorated peptide, for biomedical applications. *Int J Nanomedicine* **2018**, *13*, 2613.
[2] C. Riccardi, D. Capasso, A. Coppola, C. Platella, D. Montesarchio, S. Di Gaetano, G. N. Roviello, D. Musumeci. Synthesis, antiproliferative activity, and DNA binding studies of nucleoamino acid-containing Pt(II) complexes. *Pharmaceuticals* **2020**, *13*, 284.
[3] P. L. Scognamiglio, C. Platella, E. Napolitano, D. Musumeci, G. N. Roviello, From Prebiotic chemistry to supramolecular biomedical materials: exploring the properties of self-assembling nucleobase-containing peptides. *Molecules* **2021**, *26*, 3558.
[4] G. N. Roviello, D. Musumeci, E. M. Bucci, C. Pedone, Evidences for supramolecular organization of nucleopeptides: synthesis, spectroscopic and biological studies of a novel dithymine L-serine tetrapeptide. *Molecular bioSystems* **2011**, *7*, 1073.
[5] P. L. Scognamiglio, C. Riccardi, R. Palumbo, T. Gale, D. Musumeci, G. N. Roviello, Self-assembly of thyminyl L-tryptophanamide (TrpT) building blocks for the potential development of drug delivery nanosystems. *J Nanostruct Chem* **2024**, *14*, 335-353.

CINMPIS DAYS 2025, Keynote Lecture n. 6

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2021–Present	Associate Professor, University of Napoli Federico II, Italy
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2010–2011	Science and chemistry teacher at Napoli high schools, Italy
2009–2010	Post-doc fellowships, University of Napoli Federico II, Italy
2007–2009	R&D researcher, Bionucleon srl, company's Napoli Laboratories, Italy
2002–2007	Post-doc fellowships, IBB-CNR (National Research Council) of Napoli, Italy
2001	PhD in Chemical Sciences, University of Naples Federico II, Italy
1997	Master's degree in Chemistry, University of Naples Federico II, Italy

Research Interests:
Bioorganic chemistry, oligonucleotide aptamers, G-quadruplexes, nucleoamino acids, nucleopeptides, metal complexes, biomolecular interactions.

Selected Publications:

1. E. Napolitano, A. Criscuolo, C. Riccardi, C.L. Esposito, S. Catuogno, G. Coppola, G.N. Roviello, D. Montesarchio, D. Musumeci, Directing in vitro selection towards G-quadruplex-forming aptamers to inhibit HMGB1 pathological activity *Angew Chem Int Ed* **2024**, *63*, e202319828.
2. P.L. Scognamiglio, C. Riccardi, R. Palumbo, T. Gale, D. Musumeci, G.N. Roviello, Self-assembly of thyminyl L-tryptophanamide (TrpT) building blocks for the potential development of drug delivery nanosystems. *J Nanostructure Chem* **2023**, *14*, 335.
3. C. Platella, E. Napolitano, C. Riccardi, D. Musumeci, D. Montesarchio, Disentangling the structure-activity relationships of naphthalene diimides as anticancer G-quadruplex-targeting drugs. *J Med Chem.* **2021**, *64*, 3578.
4. C. Riccardi, D. Capasso, A. Coppola, C. Platella, D. Montesarchio, S. Di Gaetano, G.N. Roviello, D. Musumeci, Synthesis, antiproliferative activity, and DNA binding studies of nucleoamino acid-containing Pt(II) complexes. *Pharmaceuticals* **2020**, *13*, 284.
5. C. Platella, U. Raucci, N. Rega, S. D'Atri, L. Levati, G.N. Roviello, M.P. Fuggetta, D. Musumeci, D. Montesarchio, Shedding light on the interaction of polydatin and resveratrol with G-quadruplex and duplex DNA: a biophysical, computational and biological approach. *Int J Biol Macromol* **2020**, *151*, 1163.
6. D. Musumeci, V. Roviello, G.N. Roviello, DNA- and RNA-binding ability of oligoDapT, a nucleobase-decorated peptide, for biomedical applications. *Int J Nanomedicine* **2018**, *13*, 2613.
7. D. Musumeci, L. Rozza, A. Merlino, L. Paduano, T. Marzo, L. Massai, L. Messori, D. Montesarchio, Interaction of anticancer Ru(III) complexes with single stranded and duplex DNA model systems. *Dalton Trans* **2015**, *44*, 13914.
8. D. Musumeci, J. Amato, A. Randazzo, E. Novellino, C. Giancola, D. Montesarchio, B. Pagano, G-quadruplex on oligo affinity support (G4-OAS): an easy affinity chromatography-based assay for the screening of G-quadruplex ligands. *Anal Chem* **2014**, *86*, 4126.
9. D. Musumeci, G.N. Roviello, D. Montesarchio, An overview on HMGB1 inhibitors as potential therapeutic agents in HMGB1-related pathologies. *Pharmacol Ther* **2014**, *141*, 347.

KS n° 7

APPLICATION OF THE PHOTO-FRIES REARRANGEMENT REACTION IN ORGANIC SYNTHESIS

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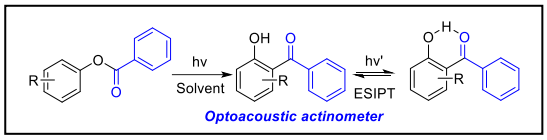
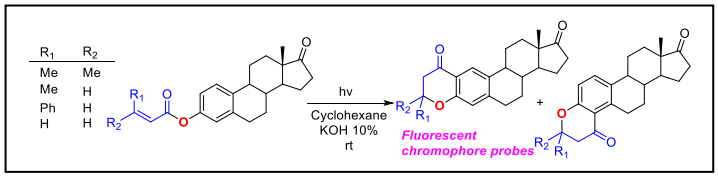
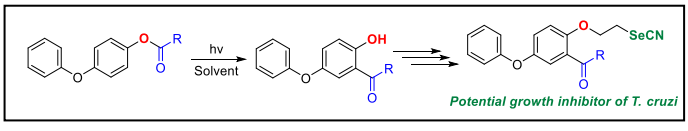
The photo-Fries rearrangement reaction is a pericyclic reaction that upon direct UV irradiation of aryl esters leads to the [1,3]- and [1,5]-acyl migration providing a wide variety of aryl phenones, interesting building blocks to be used in material chemistry, optoacoustic actinometers, fluorescent chromophore probes and compounds with potential biological properties. Three valuable synthetic approaches illustrating the application of the photo-Fries rearrangement reaction will be described. Irradiation of aryl benzoates provides a series of substituted 2-hydroxybenzophenones in modest to good yields suitable for optoacoustic actinometers. The method allows for the measuring the prompt heat released from the singlet state and synthons are used for the preparation of sunscreen. Notably, irradiation of aryl benzoates in micellar solutions enhances the photoproduct yields up to 98% due to coupling reaction of the singlet radical pairs within the hydrophobic core of the micelles.[1]





The 4-chromanone ring, a well-known oxygen heterocycle, features in a wide variety of compounds of biological and medicinal interest. Direct UV irradiation of 3-(alkenoyl) estrone (and 17-*nor*estrone) derivatives afforded substituted 4-chromanone fused steroids in good yields. This methodology involves a one-pot two consecutive pathways, *i.e.*, the photo-Fries rearrangement reaction and a based-catalyzed intramolecular *oxa*-Michael addition reaction. Potential fluorescence chromophore probes can be prepared by this method due to their lipophilicity.[2] Finally, a multistep synthetic sequence leading to the preparation of a series of 2-acyl-4-phenoxyphenoxyethyl seleno cyanate derivatives with potential biological activity against *Trypanosoma cruzi*, the causative agent of Chagas disease, has been carried out successfully involving the photo-Fries rearrangement reaction as the key step for the introduction of the acyl group in *ortho*-position bearing alkyl chains of different length and a phenyl group.[3]



[1] G. Siano, S. Crespi, M. Mella, S. M. Bonesi, *J. Org. Chem.* **2019**, *84*, 4338.
[2] M. I. Quindt, G. F. Gola, J. Ramirez, S. M. Bonesi, *J. Org. Chem.* **2023**, *88*, 13796.
[3] V. Lucena, S. H. Szajnman, J. B. Rodriguez, S. M. Bonesi, *Eur. J. Org. Chem.* **2024**, *27*, e202400201.

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1996–1998	Posdoctoral Fellowship, University of Pavia, Pavia, Italy
1995 PhD	University of Buenos Aires, Argentina
1999–Present	Member of the CONICET (Argentinean CNR)
2000–Present	Visiting Professor at the PhotoGreen Lab, University of Pavia, Italy

Research Interests:

Preparative photochemistry, photophysics, confined media, laser flash photolysis, synthesis.

Selected Publications:

1. V. Lucena, J. B. Rodriguez, S. H. Szajnamn, S. M. Bonesi, Effect of confined and micellar media on the photo-Fries reaction of 4-phenoxyphenol esters. Valuable key step toward the preparation of aryloxyethylselenocyanates *J. Org. Chem.*, **2025**, *in press*.
2. M. L. Salum, S. Protti, M. Mella, S. M. Bonesi, Effect of sustainable and confined media on the photoinduced [6p]-electrocyclization reaction of diphenyl and N-methyldiphenylamines *ChemPhotoChem*, **2024**, *10*, e202400051.
3. I. E. Romero, S. Barata Vallejos, A. Postigo, S. M. Bonesi, Perfluoroalkylation of triarylamines by EDA complexes and ulterior sensitized 6p-electrocyclization to perfluoroalkylated *endo*-Carbazoles. Mechanistic and photophysical studies. *Chemistry Eur. J.*, **2024**, e202400905.
4. M. I. Quindt, G. F. Gola, J. A. Ramirez, S. M.Bonesi, Light-driven two-step preparation of 4-chromanone fused to estrone derivatives *J. Org. Chem.*, **2023**, *88*, 13796.
5. I. E. Romero, A. Postigo, S. M. Bonesi, Solvent effects on the photoinduced [6p]-electrocyclization reactions of mono-, di- and trisubstituted arylamines. Photophysical, preparative photochemistry and mechanistic investigations *J. Org. Chem.*, **2023**, *88*, 4405.
6. M. I. Quindt, G. F. Gola, J. A. Ramirez, S. M. Bonesi, The Photo-Fries rearrangement of some 3-acyl estrone in homogeneous media. Preparative and mechanistic studies *J. Org. Chem.*, **2019**, *84*, 7051.
7. G. Siano, S. Crespi, M. Mell, S. M. Bonesi, Selectivity in the photo-Fries rearrangement of some aryl benzoates in green and sustainable media. Preparative and mechanistic studies *J. Org. Chem.*, **2019**, *84*, 4338.
8. S. M. Bonesi, S. Crespi, D. Merli, I. Manet, A. Albin, Direct irradiation of aryl sulfides. Homolytic fragmentation and sensitized S-oxidation *J. Org. Chem.*, **2017**, *82*, 9054.

KS n° 8

LIGHT AT WORK: MOLECULAR ENGINEERING OF II-CONJUGATED COMPOUNDS TOWARDS RESPONSIVE MATERIALS

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Stimuli-responsive molecular materials play a fundamental role in numerous chemical and biochemical processes in our daily lives. [1,2] Among various stimuli, light stands out as one of the most powerful and versatile options due to its selectivity and potential for use in environmentally sustainable technologies. In this context, light-responsive compounds capable of modulating their molecular structure, such as through trans-cis isomerization, are particularly appealing. These compounds not only adjust their optical activity upon excitation but can also serve as molecular actuators. [3] In this talk, we will explore the innovative application of azobenzene as a photochromic component for creating sustainable, self-tinting glass-like materials derived from wood, as well as, we will demonstrate its role as a molecular actuator for fine-tuning the π-conjugation in thiophene derivatives, paving the way for the development of environmentally friendly optoelectronic sensors. [4] The molecular architectures proposed in this work represent a new generation of light-mediated materials that not only harness the versatility of light-responsive compounds but also offer innovative solutions for sustainable technologies, particularly in the development of self-tinting materials and self-powered optoelectronic sensors.

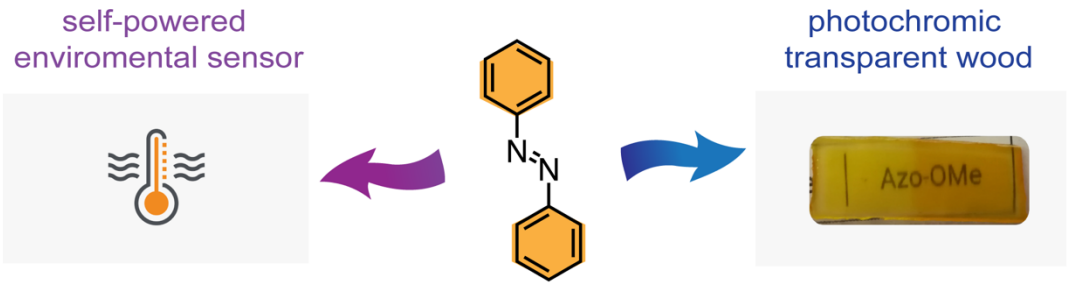

Figure 1.

[1] Y. Oaki, S. Fujii, *Chem. Commun*., **2024**, *60*, 9163–9176
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[4] A. Jozeliūnaitė, A. Rahmanudin, S. Gražulis *et al.*, *Chem. Eur. J.*, **2022**, *28*, e202202698

CINMPIS DAYS 2025, Keynote Lecture n. 8

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2023–Present	Associate Professor, University of Cagliari, Italy
2020–2022	Assistant Professor (Tenure -Track), University of Cagliari, Italy
2018–2020	(Startup) Co-founder LironiX – (Company) AC Immune
2013–2017	Junior PI, Institute of Materials, EPFL, Switzerland (SNSF Ambizione Fellow)
2011–2013	Postdoc, Dep. Chemistry, Uni. of Geneva, Switzerland (Marie Curie Fellow)
2010–2011	(6 months) Postdoc, IIT - Center for Nano Science and Technology, Italy
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Research Interests:
Organic and supramolecular chemistry, material science, optoelectronics, responsive materials.

Selected Publications:

1. A. L. Sanna, S. Acca, E. Podda, A. Mascia, A. Pintus, M. C. Aragoni, V. Lippoli, C. Ricci, P. Cosseddu, M. Arca, G. Sforazzini, Unveiling the significance of adduct formation between thiocarbonyl Lewis donors and diiodine for the structural organization of rhodanine-based small molecule semiconductors *J. Mater. Chem. C* **2024**, *12*, 11352-11360.
2. A. Jozeliūnaitė, A. Rahmanudin, S. Gražulis, E. Baudat, K. Sivula, D. Fazzi, E. Orentas, G. Sforazzini, Light-responsive oligothiophenes incorporating photochromic torsional switches *Chem. Eur. J.* ***2022***, *28*, e202202698.
3. S. Shoaee, A. L. Sanna, G. Sforazzini, Elucidating charge generation in green-solvent processed organic solar cells *Molecules* **2021**, *26*(24), 7439.
4. T. Schmaltz, G. Sforazzini, T. Reichert, H. Frauenrath, Self-assembled monolayers as patterning tool for organic electronic devices, *Adv. Mater.* **2017**, *29*, 1605286
5. J. Maciejewski, A. Sobczuk, A. Claveau, A. Nicolai, R. Petraglia, L. Cervini, E. Baudat, P. Mieville, D. Fazzi, C. Corminboeuf, G. Sforazzini, Photochromic Torsional Switch (PTS): a light-driven actuator for the dynamic tuning of π-conjugation extension *Chem. Sci.,* **2017**, *8*, 361

Patents (as sole inventor):

1. G. Sforazzini, Integrity Temperature Sensor, **2023**, WO2023248117A2
2. G. Sforazzini, Compounds for use in optical and electro-optical devices' **2016**, US15/193630.

KS n° 9

CONTINUOUS FLOW SYNTHESIS AND DERIVATIZATION OF HOMO- AND HETEROCYCLIC SYSTEMS

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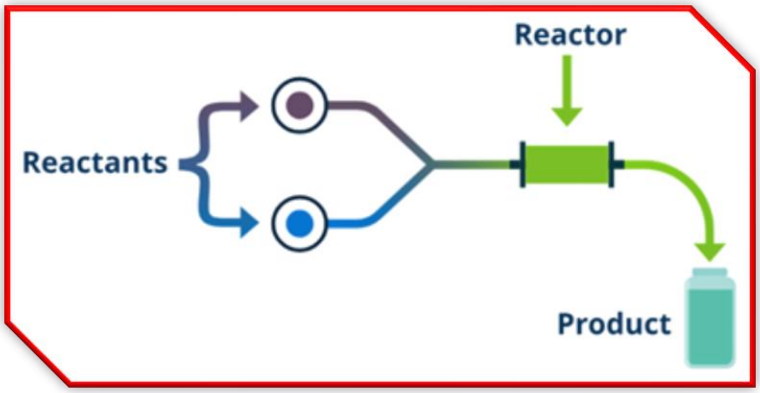
Flow chemistry is a technique of chemical synthesis involving processes conducted in continuously flowing streams rather than in batch reactors. Synthetic protocols based on this technology are gaining a growing attention due to their ability to enhance reaction efficiency, safety, and scalability. [1] Following our ongoing research concerning the synthesis and derivatization of key heterocyclic systems belonging to privileged structures, the discussion will be focused on the application of flow chemistry in procedures exploiting the reactivity of functionalized nitroalkenes and aromatic systems. Formation and derivatization of key homo and *O*-, *N*- and *S*-containing heterocycles will be presented (Figure 1). [2]



- **Pyrroles**
- **Thiophenes**
- **Isoxazoles**
- **Indoles**
- **Benzofurans**
- **Cannabinoids**

Figure 1.

[1] (a) S. Born, E. O'Neal, K. F. Jensen, *Comprehensive Organic Synthesis* **2014**, *9*, 54. (b) M. B. Plutschack, B. Pieber, K. Gilmore, P. H. Seeberger, *Chem. Rev.* **2017**, *117*, 11796.
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CINMPIS DAYS 2025, Keynote Lecture n. 9

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2007–2009	Postdoctoral fellow, University of Camerino (I)
2008	Visiting postdoctoral fellow, University of Cambridge (UK).
2007	PhD in Chemical Sciences, University of Camerino (I)

Research Interests:

Organic chemistry, heterocycles, aliphatic nitro compounds, flow chemistry, green chemistry.

Selected Publications:

1. M.E.I. Khan, T.L. Cassini, M. Petrini, A. Palmieri, Synthesis of 3,5-disubstituted isoxazoles by domino reductive nef reaction/cyclization of β-nitroenones *Org. Biomol. Chem.* **2024**, *22*, 3299-3303.
2. L. Yuan, L. Kachalova, M.E.I. Khan, R. Ballini, M. Petrin, A. Palmieri, Overcoming the usual reactivity of β-nitroenones: synthesis of 2 polyfunctionalized homoallylic alcohols and conjugated nitrotriene systems *J. Org. Chem.* **2023**, *88*, 4770-4777.
3. B. Bassetti, R. Ballini, M. Petrini, A. Palmieri, Diastereoselective conversion of β-nitro-β,γ-unsaturated ketones into conjugated (e,e)-dienones *Adv. Synth. Catal.* **2023,** *365*, 13-16.
4. A. Jorea, B. Bassetti, K. Gervasoni, S. Protti, A. Palmieri, D. Ravelli, *Adv. Synth. Catal.* **2023,** *365*, 722-727.
5. G. Lupidi, A. Palmieri, M Petrini, Sustainable and fast synthesis of fucntionalized quinoxalines promoted by Natura Deep Eutectic Solvents (NADESs) *Green Chem.* **2022**, *24*, 3629-3633.
6. E. Chiurchiù, S. Sampaolesi, P. Allegrini, D. Ciceri, R. Ballini, A. Palmieri, *Eur. J. Org. Chem.* **2021**, 1286-1289.
7. G. Lupidi, B. Bassetti, R. Ballini, M. Petrini, A. Palmieri, A new and effective one-pot synthesis of polysubstituted carbazoles starting from β-nitro-β,γ-unsaturated-ketones and indoles *Asian J. Org. Chem.* **2021**, *10*, 2334-2337.
8. E. Chiurchiù, S. Xhafa, R. Ballini, G. Maestri, S. Protti, A. Palmieri, Diastereoselective isomerization of (e)-β-nitroenones into β-nitro-β,γ-unsaturated ketones under microwave conditions *Adv. Synth. Catal.* **2020**, *362*, 4680-4686.
9. A. Palmieri, Synthesis of heterocyclic systems starting from carbonyl and carboxyl functionalized nitro compounds via one-pot processes *Eur. J. Org. Chem.* **2020**, 4247-4260.

KS n° 10

DEVELOPING NICKEL ORGANOMETALLIC NUCLEOPHILIC REAGENTS VIA PHOTOREDOX CATALYSIS

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The addition of organometallic reagents to the carbonyl group represents a key transformation, both in Academia and industry. Most of these transformations rely on a mechanism in which accessible and reactive halides are transformed into the corresponding nucleophilic organometallic reactive compounds through a redox mechanism, using a metal (Cr, Mg, Ni, etc.) in low oxidation state, by electron transfer. Using dual photoredox catalysis (metallaphotoredox catalysis), reactive nucleophilic organometallic intermediates, useful in reaction with electrophiles, can be prepared, avoiding the use of metals in low oxidation state [1]. Herein we report our research program towards the rediscovery and use of nickel organometallic reagents, introduced by Corey, Hegedus, and Semmelack many years ago. The results unveiled the extraordinary capabilities of photoredox catalysis, enabling the creation and efficient utilization of potent nucleophilic organometallic reagents under mild conditions, free from the need for strong bases or stoichiometric metal reductants. Reformatsky-type reactions, vinylation [2] and allylation [3] of aldehydes with different substituted allyls moieties will be discussed.

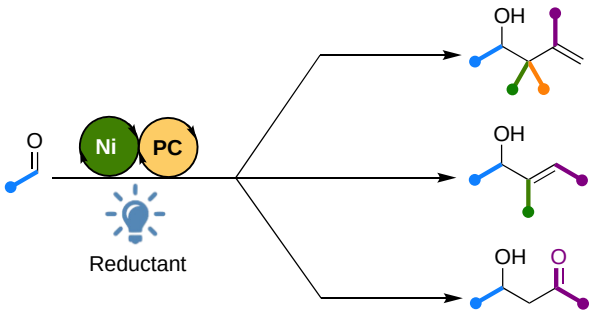

Figure 1.

[1] A. Gualandi, F. Calogero, D. Corbisiero, E. Pinosa, P. G. Cozzi, *Asian J. Org. Chem.* **2024**, *13*, e202300574.
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CINMPIS DAYS 2025, Keynote Lecture n. 10

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2022–Present	Associate Professor, University of Bologna, Italy
2016–2022	Fixed-term Assistant Professor, University of Bologna, Italy
2009–2016	Post-Doctoral Associate, University of Bologna, Italy
2008	Post-Doctoral Associate, University of Neuchâtel, Neuchâtel, Switzerland
1993 PhD	University of Bologna, Italy

Research Interests:
Photocatalysis, organic dyes, metal-catalysis, organocatalysis.

Selected Publications:

1. P.G. Cozzi, F. Calogero, L. Wilczek, E. Pinosa, A. Gualandi, R. Dorta, A. Herrera, Y. Dai, A. Rossignol, F. Negri, Z. Ziani, A. Fermi, P. Ceroni, Stable meisenheimer complexes as powerful photoreductants readily obtained from aza - heteroaromatic compounds. *Angew. Chem. Int. Ed.* **2024**, e202411074.
2. V. Giraldi, G. Magagnano, D. Giacomini, P.G. Cozzi, A. Gualandi, Photoredox-catalyzed intramolecular nucleophilic amidation of alkenes with β-lactams. *Beilstein J. Org. Chem.* **2024**, *20*, 2461–2468.
3. G. Magagnano, V. Poirier, F. Romoli, D. Corbisiero, F. Calogero, P.G. Cozzi, A. Gualandi, Dielectrophilic approach to sequential heterofunctionalization of ethylene from vinylthianthrenium salt. *Eur. J. Org. Chem*. **2024**, *27* (21), e202400224.
4. A. Fracassa, F. Calogero, G. Pavan, P. Nikolaou, A. Fermi, P. Ceroni, F. Paolucci, P.G. Cozzi, T. Scattolin, N. Demitri, F. Negri, A. Gualandi, A. Aliprandi, G. Valenti Tunable electrochemiluminescence of tadf luminophores: manipulating efficiency and unveiling water-soluble emitters. *Chem. Sci.* **2024**, *15*, 17892-17899.
5. F. Calogero, G. Magagnano, S. Potenti, F. Pasca, A. Fermi, A. Gualandi, P. Ceroni, G. Bergamini, P.G. Cozzi, Diastereoselective and enantioselective photoredox pinacol coupling promoted by titanium complexes with a red-absorbing organic dye. *Chem. Sci.* **2022**, *13*, 5973–5981.
6. F. Calogero, S. Potenti, E. Bassan, A. Fermi, A. Gualandi, J. Monaldi, B. Dereli, B. Maity, L: Cavallo, P. Ceroni, P.G. Cozzi Nickel-mediated enantioselective photoredox allylation of aldehydes with visible light. *Angew. Chem. Int. Ed.* **2022**, *61*, e202114981.
7. A. Gualandi, F. Calogero, M. Mazzarini, S. Guazzi, A. Fermi, G. Bergamini, P.G. Cozzi Cp_2TiCl_2-catalyzed photoredox allylation of aldehydes with visible light. *ACS Catal.* **2020**, *10*, 3857–3863.
8. A. Gualandi, G. Rodeghiero, A. Faraone, F. Patuzzo, M. Marchini, F. Calogero, R. Perciaccante, T.P. Jansen, P. Ceroni, P.G. Cozzi Allylation of aldehydes by dual photoredox and nickel catalysis. *Chem. Commun.* **2019**, *55*, 6838–6841.

KS n° 11

NEW TECHNOLOGIES AND GREEN PROTOCOLS FOR INDUSTRIAL CHEMICAL PROCESS INTENSIFICATION

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Although significant progress has been achieved in recent decades, the transition to greener industrial processes remains a long-term endeavour. The chemical industry plays a pivotal role in numerous value chains and serves as a key driver of innovation and new-product development. Many industrial sectors continue to suffer the inefficiencies of suboptimal energy, material and solvent usage, as well as the limited application of advanced technologies beyond the laboratory scale [1]. The gap between laboratory-scale advancements and industrial implementation remains substantial. Despite the promising results achieved with both ultrasonic and hydrodynamic cavitation techniques, their industrial application is still limited. Current industrial use is mainly observed in food extraction, processing and wastewater treatment. If these techniques were evolved into continuous flow-through systems, their potential would be maximized, leading to a revolution in extraction protocols, which are traditionally performed in batch processes. The downstream impact of sonocrystallisation and ultrasound-assisted filtration is also worthy of note. However, the widespread adoption of these innovations is often restricted by patents and proprietary industrial know-how, which limit knowledge diffusion and broader commercialization. Despite their extensive use in the food industry, the application of microwaves and radio frequencies in chemical manufacturing remains limited. The process intensification that can be achieved using dielectric heating has been demonstrated in hundreds of chemical reactions, but is particularly efficacious in heterogeneous catalysis due to its ability to provide volumetric and selective heating. Several companies now offer custom-designed industrial flow-through reactors with advanced safety features and precise process monitoring, highlighting the growing potential of the wider industrial adoption of these technologies. Mechanochemistry is another promising green technology in which the remarkable lab-scale results achieved using ball mills highlight the potential of solvent-free processes. However, scale-up entails the adapting of protocols and conditions for larger systems. Beyond a few examples of semi-continuous mechanochemical processes in ball mills, the most promising continuous-flow approach in-volves the use of reactive extruders; single-screw, twin-screw, multi-screw extruders and even sequential units can be explored to match specific synthetic targets and residence-time requirements. Regulatory agencies such as the FDA and EMA are increasingly supportive of innovation. Programs like the FDA's "Emerging Technology Program" and EMA’s "Innovation Task Force" provide guidance and early engagement with the aim of facilitating the adoption of advanced technologies. A streamlined approval pathway for continuous-flow production has also been established, highlighting the regulatory shift toward supporting greener manufacturing.

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[1] Recent author patents with industrial partners: Reactive extruders WO2024256322 A1; Subcritical water EP4173686 A2; Mechanochemistry WO2021058591 A1 and WO2018104228 A1; Ultrasound, hydrodynamic cavitation, microwaves WO 2015044411 A1; EP2520182 A1 and ES2304839 A1.

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2005–Present	Full Professor, University of Turin, Italy
2000–2005	Associate Professor, University of Turin, Italy
1994–2000	Assistant Professor, University of Turin, Italy

Research Interests:
Green chemistry, process intensification, non-conventional technologies, heterogeneous catalysis, technology transfer.

Selected Publications:

1. P. Liu, Z. Wu, M. Manzoli, G. Cravotto, Magnetic biochar generated during oil-mill wastewater treatment via microwave-assisted hydrothermal process for sonocatalytic antibiotics degradation. *J. Environ. Chem. Eng.* **2025**, *13* (1), 114996.
2. M. Salgado-Ramos, S. Tabasso, E. Calcio Gaudino, G. Cravotto, Process intensification for sustainable microwave-assisted bio *p*-cymene production from limonene. *ACS Ind. Eng. Chem. Res.* **2024**, *63* (17), 7507-7518.
3. F. Verdini, A.V. Abramova, L. Boffa, E. Calcio Gaudino, G. Cravotto, The unveiling of a dynamic duo: hydrodynamic cavitation and cold plasma for the degradation of furosemide in wastewater. *Nature Sci. Rep.* **2024**, *14* (1), 6805.
4. M. Belluati, S. Tabasso, E. Calcio Gaudino, G. Cravotto, M. Manzoli, Biomass-derived catalysts for lignocellulosic biomass and waste valorization: a circular approach. *Green Chem.* **2024**, *26*, 8642-8668.
5. E. Calcio Gaudino, M. Manzoli, M.L. Testa, V. La Parola, E. Acciardo, G. Grillo, G. Cravotto, S. Tabasso, Batch and flow green microwave-assisted catalytic conversion of levulinic acid to pyrrolidones. *ChemSusChem* **2024**, *17* (15), e202301200e202301200
6. M. Comito, R. Monguzzi, S. Tagliapietra, G. Palmisano, G. Cravotto, From batch to the continuous flow hydrogenation of pNB, pNZ-protected Meropenem. *Pharmaceutics* **2023**, *15*, 1322.

Selected Patents:

1. L. Lattuada, R. Sebastiano, G. Leonardi, G. Cravotto, A. Barge, F. Bucciol, Synthesis of non-ionic radiographic contrast agents by means of reactive extrusion. **WO2024256322 A1** 2024-12-19.
2. S. Concari, G. Cravotto, C. Cravotto, Plant and relative method for solid-liquid extraction processes in water or watery solvents in subcritical conditions **EP4173686 A2** 2023-05-033.
3. G. Cravotto, L. Jicsinszky, S. Gianni, E. Foglia, Method for the production of metal oxide pigment composite of controlled agglomerating properties. **WO2021058591 A1** 2019-09-27.

KS n° 12

USE OF SUSTAINABLE TECHNOLOGIES ENABLING DIRECT FLUOROALKYLATION AND FLUOROCARBONYLATION STRATEGIES

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The incorporation of fluorine atoms into organic molecules often leads to substantial alterations in their chemical and biological properties. As a result, organofluorine compounds have seen increasing development in synthetic methods and expanded applications in pharmaceuticals, agrochemicals, and advanced materials.[1] In our research group, a recent breakthrough in synthesizing fluorinated lithium carbenoids, which were previously difficult to access, has significantly advanced their strategic application.[2] By employing sustainable technologies as microflow devices, we have successfully prevented the decomposition of these intermediates, enabling their reactions with various electrophiles, then introducing directly a C1-F1 moiety into organic frameworks. [3] (Figure 1, a). Recently, beyond the direct nucleophilic introduction of fluoroalkyl units, we discovered that a pre-installed halodifluoromethyl group can serve as a source of fluoromethyl or fluorocarbonyl moieties via sequential cleavage of both C–F and C–X bonds (deconstructive mode).[4] Notably, the bromodifluoromethyl group acts as a C1 and F1 synthon through controlled multiple bond cleavages in the presence of amines, enabling the efficient synthesis of a wide variety of valuable nitrogen-containing compounds under basic conditions (Figure 1, b). This methodology can also be developed using mechanochemical conditions, making it more efficient and sustainable.

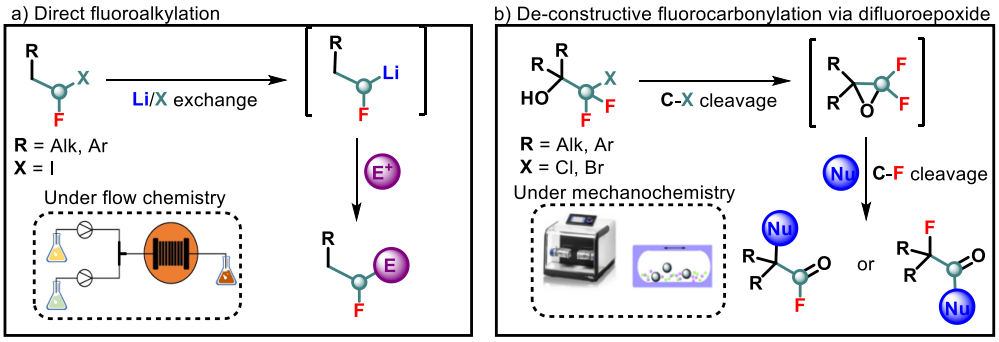

Figure 1.

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[2] G. Parisi, M. Colella, S. Monticelli, G. Romanazzi, W. Holzer, T. Langer, L. Degennaro, V. Pace, R. Luisi, Exploiting a "Beast" in carbenoid chemistry: development of a straightforward direct nucleophilic fluoromethylation strategy. *J. Am. Chem. Soc.* **2017**, *139*, 39, 13648–13651.
[3] M. Spennacchio, M. Colella, M. Andresini, R.S. Dibenedetto, E. Graziano, A. Aramini, L. Degennaro, R. Luisi, Unlocking geminal fluorohaloalkanes in nucleophilic fluoroalkylation chemistry: generation and trapping of lithiumfluorocarbenoids enabled by flow microreactors. *Chem. Commun.*, **2023**, *59*, 1373–1376.
[4] X. Ma and Q. Song, Recent progress on selective deconstructive modes of halodifluoromethyl and trifluoromethyl containing reagents. *Chem. Soc. Rev.*, **2020**, *49*, 9197-9219.

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2023–Present	Associate Professor, University of Bari "Aldo Moro", Italy
2006–2023	Assistant Professor, University of Bari "Aldo Moro", Italy
2011	Visiting researcher, Department of Synthetic Chemistry, Kyoto, Japan in collaboration with Prof. J.-i. Yoshida.
2003 PhD	University of Bari "Aldo Moro", Italy
2002	Visiting scholar at the Institute of Organic and Molecular Inorganic Chemistry, University of Groningen, under the supervision of Prof. Ben L. Feringa.

Research Interests:

Organometallic chemistry, halocarbenoids, fluorination strategies, azetidines, flow and mechanochemistry technologies.

Selected Publications:

1. E. Graziano, P. Natho, M. Andresini, F. Mastrolorito, I. Mahdi, E. Mesto, M. Colella, L. Degennaro, O. Nicolotti, R. Luisi, 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. *Adv. Synth. Cat*. **2024**, *366*, 18, 3894–3902.
2. F. Pasca, Y. Gelato, M. Andresini, G. Romanazzi, L. Degennaro, M. Colella, R. Luisi, Synthesis of alcohols: streamlined C1 to Cn hydroxyalkylation through photoredox catalysis. *Chem. Sci.* **2024**, *15*(29), 11337–11346.
3. M. Andresini, M. Colella, R.S. Dibenedetto, L. Degennaro, R. Luisi, Sustainable continuous flow synthesis of β-aminocarbonyls via acid-catalyzed hydration of N-Boc-2-azetines. *Reaction Chem. Eng*., **2023**, *8*(12), 3203–3209.
4. M. Spennacchio, M. Colella, M. Andresini, R.S. Dibenedetto, E. Graziano, A. Aramini, L. Degennaro, R. Luisi, Unlocking geminal fluorohaloalkanes in nucleophilic fluoroalkylation chemistry: generation and trapping of lithiumfluorocarbenoids enabled by flow microreactors. *Chem. Commun.*, **2023**, *59*, 1373-1376.
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6. P. Musci, T. von Keutz, F. Belaj, L. Degennaro, D. Cantillo, C.O. Kappe, R. Luisi, Flow technology for telescoped generation, lithiation and electrophilic (c3) functionalization of highly strained 1-azabicyclo[1.1.0]butanes. *Angew. Chem. – Int. Ed.*, **2021**, 60 (12), pp. 6395-6399.

KS n° 13

1,3-DIPOLAR CYCLOADDITION: A VERSATILE METHOD TO SYNTHESIZE SMALL HETEROCYCLES AND HYBRID MOLECULES

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The reaction of 1,3-dipolar cycloaddition (1,3-DC) is a powerful approach for the synthesis of a variety of five-membered heterocycles, very important scaffolds in many biological active compounds Nitrones and azides are only some of the 1,3-dipoles employed to build variable heterocyclic structures. For example, the cycloaddition of nitrones with olefins is one of the most versatile protocol for the construction of isoxazolidines, *N*,*O*-heterocycles with several stereocenters [1]. In alternative, the employment of azides as dipole and alkynes or alkenes as dipolarophiles furnishes 1,2,3-triazoles, five-membered *N*-heteroaromatic compounds with three nitrogen atoms in the ring [2]. Recently, hybrid molecules represent new potential drugs based on the combination of different pharmacophoric moieties in the same molecular skeleton, such as triazoles, pyrazoles, pyrimidines and so on, to produce a new compound with improved biological activity and lower risk of drug-drug interactions, reduced side effects with the organism and minimized drug resistance of pathogens [3]. The 1,3-dipolar cycloaddition can give an important contribute to construct hybrids with particular heterocyclic *core*.

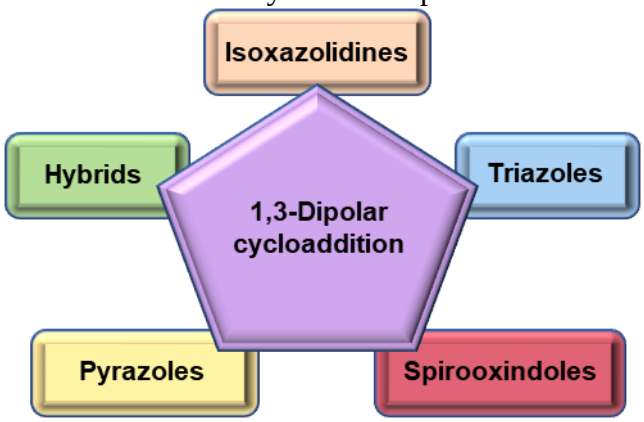

Figure 1.

In this contest, we present the synthetic strategies to prepare a variety of molecules, starting from small heterocycles such as isoxazolidines, spirooxindoles, triazoles and pyrazoles until to arrive to very complex hybrids, projected and obtained by exploiting our expertise in this field (Figure 1). Finally, biological results of the most relevant compounds will be presented.

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CINMPIS DAYS 2025, Keynote Lecture n. 13

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2022-Present	Associate Professor, University of Calabria, Italy
2005-2021	Researcher, University of Calabria, Italy
2000-2004	Postdoctoral research assistant, University of Calabria, Italy
1999 PhD	University of Calabria, Italy

Research Interests:

Heterocyclic synthesis, 1,3-dipolar cycloadditions, polymeric materials, biomaterials from waste.

Selected Publications:

1. V. Algieri, A. Tursi, P. Costanzo, L. Maiuolo, A. De Nino, A. Nucera, M. Castriota, O. De Luca, M. Papagno, T. Caruso, S. Ciurciù, G.A. Corrente, A. Beneduci, Thiol-functionalized cellulose for mercury polluted water remediation: synthesis and study of the adsorption properties. *Chemosphere* **2024**, *355*, 141891-141904.
2. V. Algieri, C. Algieri, P. Costanzo, G. Fiorani, A. Jiritano, F. Olivito, M.A. Tallarida, F. Trombetti, L. Maiuolo, A. De Nino, S. Nesci, Novel regioselective synthesis of 1,3,4,5-tetrasubstituted pyrazoles and biochemical valuation on F1FO-ATPase and mitochondrial permeability transition pore formation. *Pharmaceutics* **2023**, *15*, 498-517.
3. M.A. Tallarida, F. Olivito, C.D. Navo, V. Algieri, A. Jiritano, P. Costanzo, A. Poveda, M.J. Moure, J. Jiménez-Barbero, L. Maiuolo, G. Jiménez-Osés, A. De Nino, Highly diastereoselective multicomponent synthesis of spirocyclopropyl oxindoles enabled by rare-earth metal salts. *Org. Lett.* **2023**, *25*, 17, 3001–3006.
4. F. Olivito, V. Algieri, M.A. Tallarida, A. Jiritano, P. Costanzo, L. Maiuolo, A. De Nino, High yield synthesis of HMF from glucose and fructose by selective catalysis with water-tolerant rare earth metal triflates assisted by choline chloride. *Green Chem.* **2023**, *25*, 1679–1689.
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6. V. Algieri, C. Algieri, L. Maiuolo, A. De Nino, A. Pagliarani, M.A. Tallarida, F. Trombetti, S. Nesci, 1,5-Disubstituted-1,2,3-triazoles as inhibitors of the mitochondrial Ca^{2+}-activated F1FO-ATP(hydrol)ase and the permeability transition pore. *Ann. N.Y. Acad. Sci.* **2021**, *1485*, 43–55.
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KS n° 14

SELF-ASSEMBLY OF SUPRAMOLECULAR POLYMERS BASED ON IONIZABLE BIS-PILLAR[5]ARENE MONOMERS FOR SENSING APPLICATIONS

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Supramolecular polymers are macromolecular assemblies composed of monomeric units held together by non-covalent, reversible interactions [1]. The resulting aggregates often conjugate the properties of both classical covalent polymers and self-assembled systems, ultimately producing smart materials with stimuli-responsiveness or adaptive abilities, sometimes capable of outperforming classical polymers in sensing, delivery or materials science applications.
The supramolecular polymerization of bis-pillar[5]arene dicarboxylic acid monomers (**H9**, **H12**) has been assayed in the presence of complementary bis-guests such as 1,12-diaminododecane (**G**) or alkylidene-bis-imidazole (**G1**), yielding stimuli-responsive polymers **H12**/**G** [2] and **H9**/**G1** [3]. Furthermore, bis-pillar[5]arene **H9**, in the presence of a mixture of alkylidene- and perylene-bisimide-bis-imidazole (**G1** and **G2**, respectively), yields AA/BB-type supramolecular copolymer **H9**/**G1**/**G2** that retains the properties of the parent bi-component systems, that is, **H9**/**G1** adaptability and solubility and the photoresponsiveness of the **H9**/**G2** complex [3]. Results on the sensing and delivery applications of the **H9**, **H9**/**G1** and the **H9**/**G1**/**G2** supramolecular systems –either in solution or as water-dispersible, CTAB-microemulsified nanoparticles– will also be discussed.

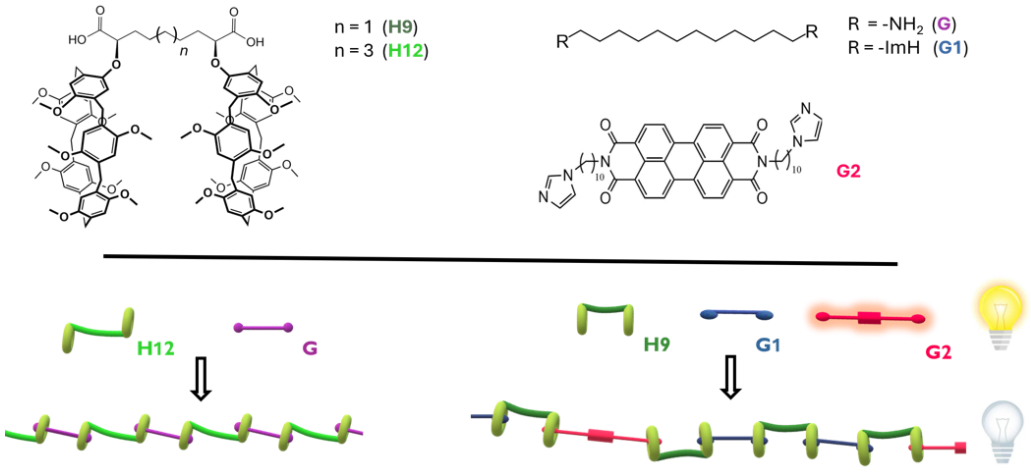

Figure 1.

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[2] A. Notti, I. Pisagatti, F. Nastasi, S. Patanè, M. F. Parisi, G. Gattuso, *J. Org. Chem.*, **2021**, *86*, 1676.
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CINMPIS DAYS 2025, Keynote Lecture n.14

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2014–2021	Associate Professor, Università degli Studi di Messina, Italy
1999–2014	Assistant Professor, Università degli Studi di Messina, Italy
1997 PhD	University of Birmingham, UK

Research Interests:
Host-guest chemistry, macrocycles, supramolecular polymers, phenolics, bioactive compounds.

Selected Publications:

1. M. Mazzaferro, D. Crisafulli, F. Mancuso, M. Milone, F. Puntoriero, A. Irto, S. Patanè, V. Greco, A. Giuffrida, I. Pisagatti, A. Notti, M.F. Parisi, G. Gattuso, A pillar[5]arene-based three-component supramolecular copolymer for the fluorescence detection of spermine. *Org. Chem. Front.* **2024**, *11*, 6293–6303.
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KS n° 15

EXPLORING PRISMARENE: AN EMERGING MACROCYCLIC HOST IN SUPRAMOLECULAR CHEMISTRY

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Prismarenes [1] represent a novel class of macrocyclic hosts synthesized through a templated approach involving thermodynamically controlled macrocyclizations [1,2,3,4,5]. These deep-cavity macrocycles, consisting of 1,5-methylene bridged 2,6-dialkoxynaphthalene units, exhibit planar chirality and possess a π-electron-rich aromatic cavity, which is crucial for defining their unique supramolecular properties [6]. Numerous studies from our group and other researchers globally have underscored the intriguing capabilities of these macrocycles in molecular recognition across both aqueous and organic solvents [5,6,7]. Notably, water-soluble anionic prismarenes can form endo-cavity complexes with neutral organic and hydrophilic pollutants in aqueous environments [7]. The stability of these complexes is significantly influenced by the displacement of constrained water molecules from the prismarene's cavity and the hydrogen bonding interactions facilitated by water between the host and guest molecules [7].

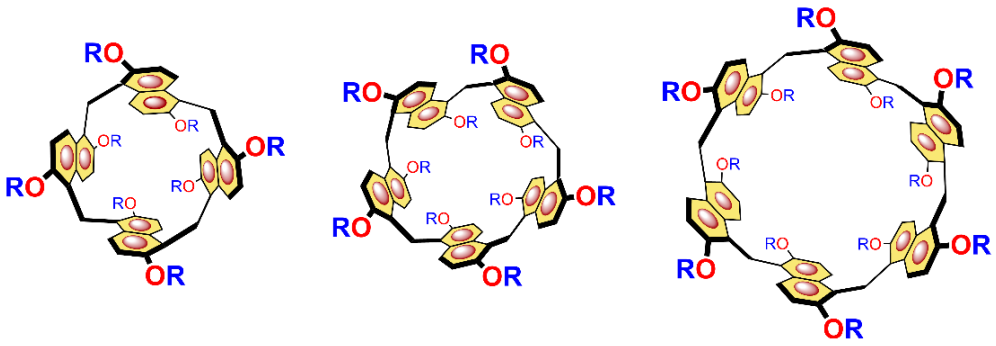

Figure 1.

[1] P. Della Sala, R. Del Regno, C. Talotta, A. Capobianco, N. Hickey, S. Geremia, M. De Rosa, A. Spinella, A. Soriente, A. Spinella, P. Neri, C. Gaeta, *J. Am. Chem. Soc.* **2020**, *142*, 1752–1756. Highlighted in: L.-P. Yang, W. Jiang, *Angew. Chem. Int. Ed*. **2020**, *7*, 15794–15796.
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[3] Del Regno, R.; Della Sala, P.; Vollono, I.; Talotta, C.; Neri, P.; Hickey, N.; Joshi, S.; Geremia, S.; Gaeta, C. *Org. Chem. Front*., **2024**, *11*, 2710–2719.
[4] R. Del Regno, G. D. G., Santonoceta, P. Della Sala, M. De Rosa, A. Soriente, C. Talotta, A. Spinella, P. Neri, C. Sgarlata, C. Gaeta, *Org. Lett*., **2022**, *24*, 2711−2715.
[5] R. Del Regno, A. Palmieri, P. Della Sala, C. Talotta, M. De Rosa, G. Campanile, C. Argenio, C. Gaeta, *Org. Lett*. **2024**, *39*, 8228−8232.
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CINMPIS DAYS 2025, Keynote Lecture n. 15

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2023–Present	Full Professor, University of Salerno, Italy
2014–2023	Associate Professor, University of Salerno, Italy
2004–2014	Assistant Professor, University of Salerno, Italy
2005	Visiting researcher, Johannes Gutenberg University Mainz, Germany
2005 PhD	University of Salerno, Italy

Research Interests:
Supramolecular chemistry, molecular recognition, new macrocycles, supramolecular catalysis.

Selected Publications:

1. P. Della Sala, R. Del Regno, C. Talotta, A. Capobianco, N. Hickey, S. Geremia, M. De Rosa, A. Spinella, A. Soriente, A. Spinella, P. Neri, C. Gaeta, Prismarenes: a new class of macrocyclic hosts obtained by templation in a thermodynamically controlled synthesis. *J. Am. Chem. Soc*., **2020**, *142*, 1752–1756.
2. P. Della Sala, R. Del Regno, L. Di Marino, C. Calabrese, C. Palo, C. Talotta, S. Geremia, N. Hickey, A. Capobianco, P. Neri, C. Gaeta, An intramolecularly self-templated synthesis of macrocycles: self-filling effects on the formation of prismarenes. *Chem. Sci*., **2021**, *12*, 9952−9961.
3. R. Del Regno, G. D. G., Santonoceta, P. Della Sala, M. De Rosa, A. Soriente, C. Talotta, A. Spinella, P. Neri, C. Sgarlata, C. Gaeta, C. molecular recognition in an aqueous medium using water-soluble prismarene hosts. *Org. Lett.*, **2022**, *24*, 2711−2715.
4. R. Del Regno, P. Della Sala, I. Vollono, C. Talotta, P. Neri, N. Hickey, S. Joshi, S. Geremia, C. Gaeta, Synthesis, conformational properties, and molecular recognition abilities of novel prism[5]arenes with branched and bulky alkyl groups. *Org. Chem. Front*., **2024**, *11*, 2710–2719.
5. R. Del Regno, P. Della Sala, D. Picariello, C. Talotta, A. Spinella, P. Neri, C. Gaeta, *per*-hydroxylated prism[n]arenes: supramolecularly assisted demethylation of methoxy-prism[5]arene. *Org. Lett.*, **2021**, *23*, 8143−8146.
6. R. Del Regno, P. Della Sala, G. D. G. Santonoceta, P. Neri, M. De Rosa, C. Talotta, C. Sgarlata, A. De Simone, C. Gaeta, Under the influence of water: molecular recognition of organic hydrophilic molecules in water with a prismarene host driven by hydration effects. *Chem. Eur. J*. **2024**, *30*, e202401734.
7. R. Del Regno, A. Palmieri, P. Della Sala, C. Talotta, M. De Rosa, G. Campanile, C. Argenio, C. Gaeta, Thermodynamically templated macrocyclizations: enhancing the synthesis of prism[5]arenes with tailor-made guests. *Org. Lett*. **2024**, *26*, 8228−8232.
8. P. Della Sala, R. Del Regno, V. Iuliano, A. Capobianco, C. Talotta, S. Geremia, N. Hickey, P. Neri, C. Gaeta, Confused-prism[5]arene: a conformationally adaptive host by stereoselective opening of the 1,4-bridged naphthalene flap. *Chem. Eur. J.,* **2023**, *29*, e202203030.

KS n° 16

SUSTAINABLE SYNTHETIC METHODOLOGIES FOR THE SYNTHESIS OF HETEROCYCLIC COMPOUNDS

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Among the top 200 best-selling drugs of 2023, approximately 44% are small molecules, many of which are heterocyclic compounds. This highlights the crucial role that heterocycles play in modern drug development. The growing emphasis on sustainability within the industrial chemistry value chain has driven the pursuit of innovative and efficient synthetic methodologies designed to enable the cost-effective and eco-friendly production of these crucial structural motifs. We outline our strategies for designing protocols to synthesize O- and N-heterocycles, adhering to Green Chemistry principles to minimize the environmental impact. Central to this approach is the choice of methodologies that maximize atom economy and minimize waste generation. Notable among these are click reactions for the synthesis of 1,2,3-triazoles [1, 2] and C–H functionalization methods. Our efforts focus on leveraging C–H functionalization to enable the synthesis of coumarins and carbazoles. [3, 4] Our approach employs heterogeneous metal catalysts, facilitating recycling and reducing metal leaching paired with a recoverable reaction medium or bio-derived solvents. Scalability is crucial, leveraging flow techniques as a key tool. The choice of starting materials is considered; phenols are a class of potential-lignin-derived starting materials, and their valorization into value-added products is of great interest.

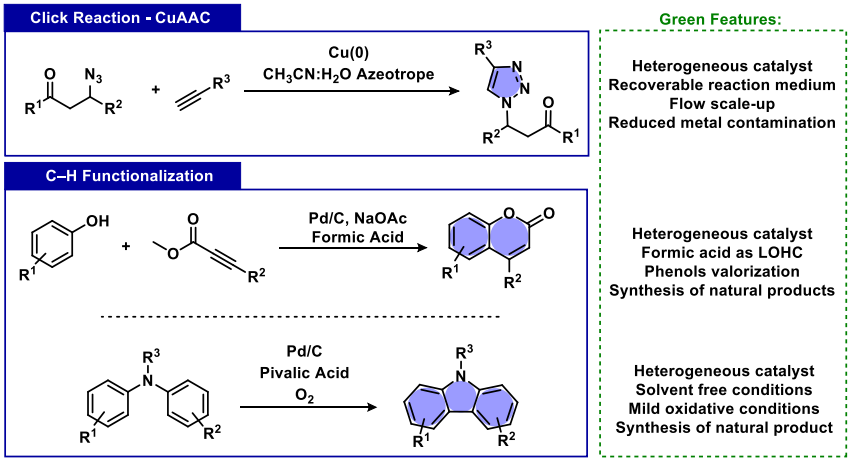

Figure 1.

[1] G. Brufani, F. Valentini, G. Rossini, L. Carpisassi, D. Lanari, L. Vaccaro *Green Chem.*, **2023**, *25*, 2438-2445
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CINMPIS DAYS 2025, Keynote Lecture n. 16

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2024–Present	PostDoc, Università Mediterranea Reggio Calabra Dipartimento Ingegneria Civile, Energia, Ambiente e Materiali
2021–2024	PhD, Università degli Studi di Perugia, Dipartimento di Chimica Biologia e Biotecnologie
2023	Visiting PhD Student, McGill University, Montréal, Canada

Research Interests:
Sustainable and eco-friendly synthetic methodologies, heterogeneous catalysis, flow chemistry.

Selected Publications:

1. G. Brufani, B. Di Erasmo, C.J. Li, L. Vaccaro, Csp2–H functionalization of phenols: an effective access route to valuable materials via Csp2–C bond formation, *Chem. Sci.*, **2024**, *15*, 3831-3871.
2. G. Brufani, S. Chen, B. Di Erasmo, A. Maria Afanasenko, Y. Gu, C.-J. Li, L.Vaccaro, A sustainable access route to carbazoles via C H/C H oxidative functionalization/cyclization of arylamines, *ACS Sustainable Chem. Eng.* **2024**, *12*, 22, 8562–8572.
3. G. Brufani, F. Valentini, F. Sabatelli, B. Di Erasmo, A. Maria Afanasenko, C.-J. Li, L. Vaccaro, Valorisation of phenols to coumarins through one-pot palladium-catalysed double C–H functionalizations - HOT Green Chemistry article *Green Chem.*, **2022**, *24*, 9094-9100.
4. F. Ferlin, G. Brufani, G. Rossini, L. Vaccaro, Classic vs. C–H functionalization strategies in the synthesis of APIs: a sustainability comparison *Green Chem.*, **2023**, *25*, 7916-7933.
5. G. Brufani, F. Valentini, G.Rossini, L. Carpisassi, D. Lanari, L.Vaccaro, Continuous flow synthesis of 1,4-disubstituted 1,2,3-triazoles via consecutive β-azidation of α,β-unsaturated carbonyl compounds and CuAAC reactions *Green Chem.*, **2023**, *25*, 2438-2445.
6. F. Valentini, G. Brufani, G. Rossini, F. Campana, D. Lanari, L. Vaccaro, POLITAG-MF as Heterogeneous Organocatalyst for the Waste-Minimized Synthesis of β-Azido Carbonyl Compounds in Batch and under Flow Conditions *ACS Sustainable Chem. Eng.* **2023**, *11*, 7, 3074–3084.
7. G. Brufani, F. Valentini, G. Rossini, L. Rosignoli, Y. G., P. Liu, L. Vaccaro, Waste-minimized continuous flow copper-catalyzed azide-alkyne cycloaddition with low metal contamination Green *Synthesis and Catalysis* **2023**, *4*, 154–159.

Oral Communications

OC n° 1

SURFACE MODIFICATION OF NANOCELLULOSE TOWARDS ADDITIVE MANUFACTURING

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In recent years, nanocellulose has emerged as one of the most promising bio-based materials for use in many fields, spacing from biomedical to additive in polymers, thanks to its ability to enhance the mechanical properties of resulting nanocomposites. However, the inherent hydrophilicity of nanocellulose significantly hinders its dispersion within lipophilic media, creating major challenges in both cellulose loading and final performance. To address this issue, we synthesized a series of nanocomposites designed for vat photopolymerization, utilizing a commercial resin combined with nanocellulose modified with fatty acids derived from safflower oil (SOFA). This modification effectively hydrophobized the cellulose crystals, enabling their uniform dispersion within the polymeric resin. This innovative approach facilitates the production of solid, intricate objects without structural defects, using bio-based nanocomposites with CNCs-SOFA concentrations of up to 5 wt%. Additionally, mechanical and optical property analyses revealed that CNCs-SOFA nanocomposites exhibit enhanced stiffness and strength while maintaining a high level of transparency compared to the unmodified resin. [1]

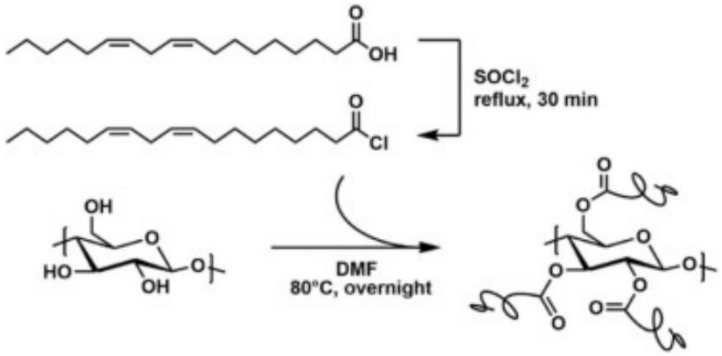

Figure 1.

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OC n° 2

DISCLOSING THE PROPERTIES OF SILK FIBROIN IN HETEROGENEOUS CATALYSIS

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The global demand for sustainable development has highlighted the need to explore new materials for several applications, including catalysis. Among the promising candiPresents, biopolymers have gained significant attention as an eco-friendly alternative to synthetic polymers in catalysis. In fact, their natural abundance, remarkable chemical efficiency, and environmentally beneficial properties, such as biodegradability and non-toxicity, make biopolymers a compelling choice for developing sustainable catalytic systems. [1] Silk, one of the most valuable natural fibers, exemplifies the potential of biomaterials. [2] Renowned for its exceptional mechanical properties, silk combines strength, flexibility, and toughness in a manner unmatched by other natural or synthetic materials, making it a subject of considerable interest for diverse applications, including biomedicine, optoelectronics and many other technological applications. [3] Silk fibroin (SF) is constituted mainly by glycine (46%), alanine (30%), serine (12%) and other amino acids in smaller percentages. [4] Such amino acids of SF are able of coordinating metals mainly thanks to the presence of oxygen and nitrogen atoms, that already demonstrated their ability to bind metal ions through highly coordinated structures. [5]

Taking advantage of this property, the present study explores the potential of SF as a support for heterogeneous metal catalysis. Specifically, we report the development of new heterogeneous catalyst with metal supported on SF, highlighting an outstanding catalytic activity. [6]

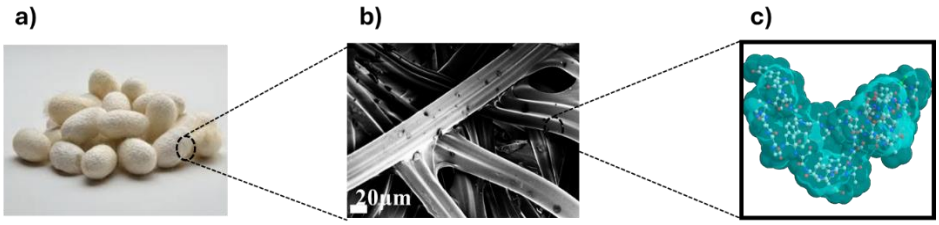

Figure 1. a) *Bombyx mori* cocoons b) SEM image of SF fibers c) Solvent accessible surface.

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OC n° 3

LIGHTING UP TYROSINASE INHIBITORS

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Tyrosinase (TYR, EC 1.14.18.1) is a copper-containing enzyme widely distributed in nature that catalyzes two reactions in the melanin synthesis: *i)* the hydroxylation of tyrosine to L-DOPA the so called "monophenolase activity" and ii) the subsequent oxidation of L-DOPA to dopaquinone *alias* the "diphenolase activity".[1] The level of tyrosinase is closely related to different esthetic issues (such as hyperpigmentation of skin or vitiligo),[2] is related to dopamine neurotoxicity and neurodegeneration, associated with Parkinson's disease [3] and can be regarded as an important biomarker of melanoma cancer [4], a fatal skin carcinoma with poor diagnosis and high metastasis features. Detection of TYR with high sensitivity has a great importance for observing its activities in biological processes but also for clinical diagnosis.[5] Furthermore, the possibility of inhibiting TYR activities, could be useful in medicine to treat disorders and diseases associated with the accumulation of melanin. Numerous studies have identified both synthetic and natural inhibitors of TYR such as kojic acid, flavonoids, curcuminoids, thioureas and other heterocyclic compounds. Among them we paid our attention on 4-(4-hydroxyphenyl)piperazine-based compounds [6] which have proven to be more effective than the reference compound kojic acid with a competitive mechanism of inhibition towards diphenolase activity of *Agaricus bisporus Tyrosinase* (AbTyr). Here we present the design and synthesis of luminescent 4-(4-hydroxyphenyl)piperazine-derivatives (*e.g.* BODIPY, curcumin and porphyrin) and the results of studies on their interactions with TYR *in silico*, *in vitro* and *in vivo*.

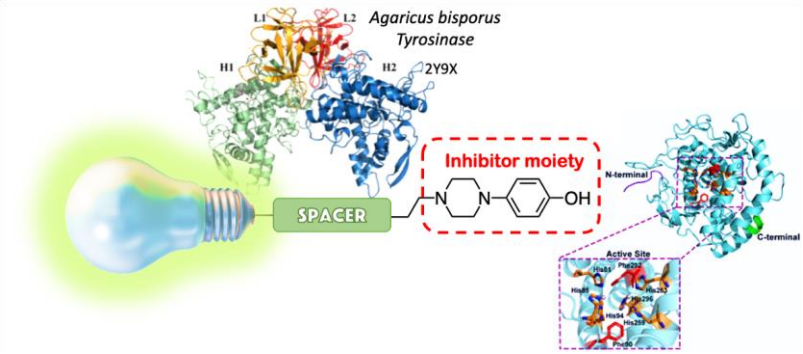

Figure 1.

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OC n° 4

DISCOVERY OF NEW LEUKEMIA INHIBITORY FACTOR RECEPTOR ANTAGONISTS: 4,9-ESTRADIEN-3-ONE SCAFFOLD

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Leukemia inhibitory factor (LIF) is a regulatory factor belonging to IL-6 family of cytokines, which is involved in different activities cell-type specific: cell proliferation, the induction or suppression of the differentiation, and the induction of mature cell function. Indeed, as other cytokine of IL-6 family, LIF plays a prominent role in inflammation, autoimmunity, and cancer. [1] Different studies show that LIF promotes the progression and metastasis of tumors. LIF acts on target cells by activating a heterodimeric cell membrane receptor (LIFR) made up by LIFRβ, a low-affinity subunit, and the glycoprotein (gp)-130, the signal transducer subunit. Recent studies have shown that LIF/LIFR are highly expressed in solid tumors. The downstream signaling of the LIF/LIFR pathway involves a Janus Kinase (JAK)-1-induced STAT3 phosphorylation [2]. Thus, the inhibition of LIFR signalling could have beneficial effects on cell growth and tumour progression in several cancers.

In 2019, a novel study identified a first-in-class inhibitor of LIFR, EC359, which directly interacts with LIFR to block LIF/LIFR axis. Starting from this study, first we developed an *in silico* strategy to identify potential LIFR antagonists. This work allowed the identification of mifepristone as potential LIFR antagonist [3]. Due to its antiprogestinic effect, mifepristone is not able to be used as an antitumoral drug. This steroid is an attractive starting point since the compound demonstrates versatility with respect to functional group manipulation at the 11- and 17-positions on the steroidal backbone, which could provide valuable SAR [4].

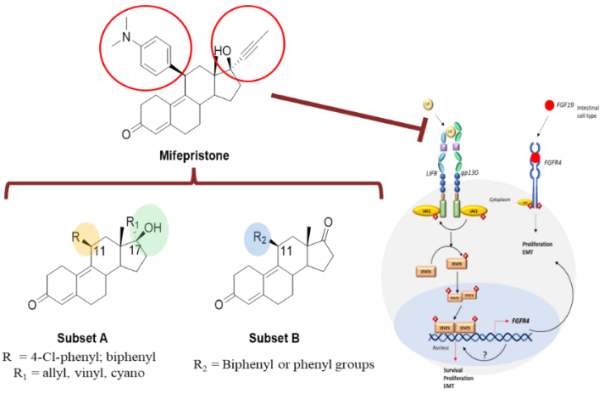

Figure 1. General structures of Mifepristone derivatives.

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OC n° 5

THE DUAL ROLE OF TEMPO IN ELECTROOXIDATIVE ALLENE DIOXYGENATION

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The unique reactivity of allenes, arising from their cumulated π systems, has made them invaluable intermediates in organic synthesis. Despite their potential, electrochemical transformations of allenes remain underexplored. In this communication we will delve into the electrooxidative dioxygenation of allenes mediated by tetramethylpiperidine *N*-oxyl (TEMPO).[1] Using a combination of techniques like CV, ReactNMR, and DFT calculations, we undisclosed the dual role of TEMPO as both an electron mediator and a reactant.[1]

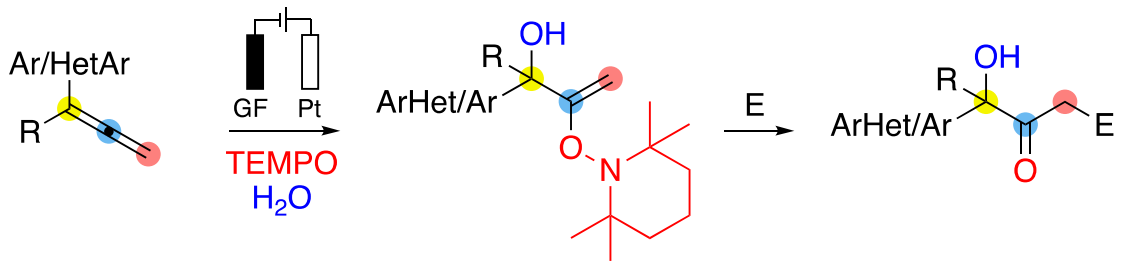

Figure 1.

The study reveals an outer-sphere electron transfer by $TEMPO^+$, enabling selective hydroxylation and vinyl-TEMPO formation. Optimization of reaction conditions achieved yields of up to 71%, with mechanistic studies revealing key factors influencing regioselectivity and chemoselectivity.[1] The synthetic utility of this methodology is demonstrated through postfunctionalization of the vinyl-TEMPO products into α-heteroatom ketones and other value-added compounds.[1]

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OC n° 6

DEVELOPMENT OF GRAPHENE-BASED SOLID SORBENTS FOR CO_2 CAPTURE

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The increasing consumption of fossil fuels and the rapid rise in atmospheric CO_2 concentrations highlight the urgent need for energy-efficient and selective methods to capture CO_2[1]. Recently, graphene-based materials have been proposed as effective CO_2 adsorbents due to their planar geometry, large surface area, versatile surface chemistry, and tunable structure[2,3].

In this study, we developed two nanoporous graphene oxide (nGO) systems: one derived from industrial graphite waste and the other from commercial graphene oxide. Both nGO materials were modified with tetraethylene pentamine (nGO-TEPA) to introduce amino groups, which are known for their strong affinity for CO_2. We characterized their structure, morphology, and chemical composition using micro-Raman spectroscopy, X-ray photoelectron spectroscopy, thermogravimetric analysis, and scanning electron microscopy. To assess their capacity for CO_2 adsorption and release, adsorption tests are currently in progress. The first experimental results indicated the higher absorption capacity of the two nanoporous derivatives, with adsorption values of 2% and 2.2% under conditions of room pressure and temperature, respectively. However, under room temperature and a pressure of 20 bar, the same materials exhibited significantly higher adsorption values of 10% and 13%, respectively. Additionally, *in vivo* toxicity tests conducted on zebrafish larvae demonstrated no cytotoxic effects at the final concentration of 25µg/ml, for all graphene derivatives.

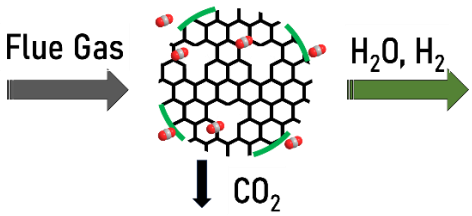

Figure 1. Representation of CO_2 molecules absorbed on the nGO-TEPA sample.

Funding: PRIN PNRR project CHARYBDIS (Carbon-High AdsoRption bY Bi-functionalizeD solId Sorbents, MESSINA, CUP J53D23014730001), funded by the European Union – Next Generation EU.

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OC n° 7

FASCINATING PLOY TO THE CONTROLLED ORTHOGONALIZATION OF WATER-SOLUBLE NAPHTHALENE DIIMIDES

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The broad aromatic surface and advantageous optoelectronic properties of naphthalene diimides (NDIs) make them a versatile foundation for designing molecules across fields such as materials science, supramolecular chemistry, and biological and medical research applications.[1] A particularly noteworthy aspect of water-soluble NDIs (wsNDIs) is their relevance in medicinal chemistry, especially due to their strong interactions with nucleic acids, including non-canonical secondary structures like G-quadruplexes.[2] Although wsNDIs exhibit significant stability in organic solvents or acidic aqueous environments, they are prone to hydrolysis under basic conditions. Hydroxide-catalyzed hydrolysis occurs stepwise, initially forming the mono-imide (NMI), which subsequently undergoes further hydrolysis to yield diacid-diamide derivatives.[3] While imide substituents influence hydrolytic stability, their impact on the optoelectronic properties of wsNDIs is minimal. In this work, we investigated how modifications to the π-system through functionalization of the naphthalene core could influence the optoelectronic and redox properties of wsNDIs. We synthesized di-, tri-, and tetra-substituted wsNDIs, varying the substituents from bromine to amines, commonly present in known wsNDIs. Core substitution with bromine significantly enhanced hydrolysis under mild conditions with unexpected regioselectivity, leading to the selective formation of NMI intermediates. Acidification of these intermediates resulted in the formation of a diacid-imine structure, a crucial step in achieving a controlled asymmetric diimide (Scheme 1). This discovery presents an efficient new approach for the synthesis of asymmetric tetra-substituted wsNDIs, enabling the precise and selective orthogonal insertion of substituents.

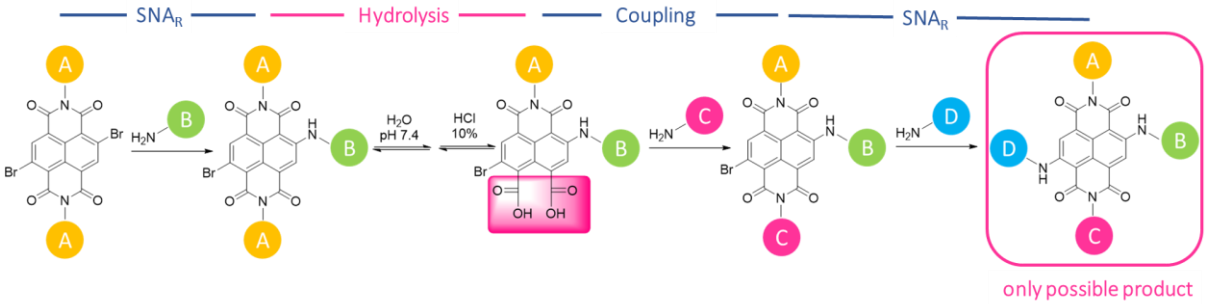

Figure 1. Schematic representation of structurally selective orthogonalization of wsNDIs

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OC n° 8

STUDIES TOWARDS THE SYNTHESIS OF VISMIONE E

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Vismione E is a natural compound belonging to the anthranoid class, which was isolated from *Psorospermum febribugum* berries [1] and from *Aspergillus* sp.[2] Vismione E exhibited a potent anticancer activity against Hedgehog pathway-dependent tumors as medulloblastoma cancer cells (Gli1 transcriptional factor inhibitor),[3] and against human breast cancer MCF-7 and human prostate PC-3 cell lines.[2]
The low yield of vismione E from extraction and purification processes of plant material, along with the difficulties in retrieving the *P. febrifugum* berries and in the complex isolation procedure, render vismione E not easily available for further biological investigations. For this reason, and since no total synthesis of vismione E have been reported so far, we decided to design a synthetic strategy towards vismione E (see Figure 1), which is based on a convergent plan inspired to the total synthesis of atrochrysone and torosachrysone, two similar preanthrones.[4] Protected vismione E could be obtained from a tandem coupling/cyclization reaction of fragment A with fragment B under basic conditions (Figure 1). Herein we reported the progress made in the total synthesis of vismione E, starting from commercially available acetylacetone and ethyl orsellinate.

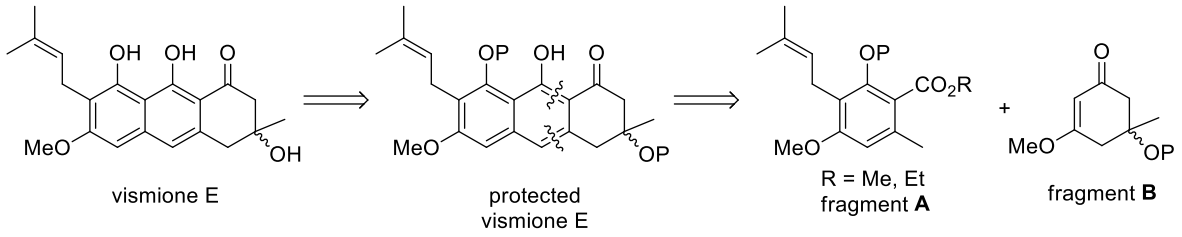

Figure 1. Retrosynthetic plan for the preparation of vismione E.

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OC n° 9

ONE-POT TWO-STEP CHEMOENZYMATIC DERACEMIZATION OF SECONDARY ALCOHOLS IN IRON-BASED DEEP EUTECTIC SOLVENTS

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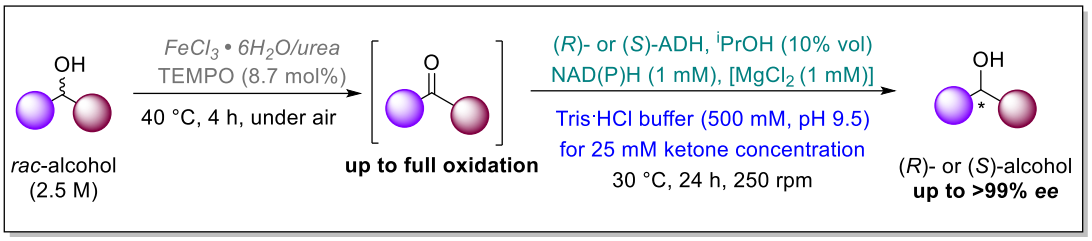
Deracemization allows the direct conversion of a racemic mixture into a single enantiomer without the need for intermediate isolation. [1] This method has sparked renewed interest in asymmetric synthesis due to its exceptional atom economy and high efficiency to produce, for instance, chiral amines or alcohols. [2] Particularly, the most common approach for the deracemization of alcohol consists of the non-selective oxidation of the hydroxyl moiety, and subsequent one-pot bioreduction of the ketone intermediate. Specifically, it involves the direct transformation of a racemic alcohol into an enantiopure alcohol through a sequence of enantioselective oxidation and reduction steps. Building on our interest in combining metal catalysis with biocatalysis, [3–5] we explored the development of a deracemization method for secondary alcohols using iron-based deep eutectic solvents (Scheme 1).



Scheme 1. Deracemization of racemic alcohols in a $FeCl_3 \cdot 6H_2O$/urea mixture.

This process demonstrated the feasibility of employing $FeCl_3 \cdot 6H_2O$/urea (2:1 mol/mol) as the reaction medium for the oxidation step, achieving a range of ketones with both electron-withdrawing and electron-donating groups, with yields varying from 26% to >99%, following a procedure previously optimized by our research group. [6] In the subsequent step performed in one-pot after intermediate dilution the resulting ketones were reduced using alcohol dehydrogenases (ADHs) exhibiting Prelog (*Lb*ADH and evo 1.1.200) or anti-Prelog (ADH-A) selectivity depending on the enzyme of choice. This one-pot two-step sequential approach produced optically active alcohols with enantiomeric excess (*ee*) values up to >99%.

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OC n° 10

TACKLING OPERATIVE CHALLENGES IN THE INDUSTRIAL PHARMACEUTICAL MANUFACTURING PROCESSES FRAMEWORK

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Therapeutic peptides market showed an impressive boost in the latest years after the pivotal approval of Glucagon Like Peptide 1 (GLP-1) analogs for the treatment of diabetes and, more importantly, weight control [1].
This market explosion opened the worldwide search of innovative manufacturing processes able to produce multi-Kg batches with high level of quality at a competitive price.
To achieve this task, all technical challenges must be addressed to improve productivity and ensure cost effectiveness, comprising those related to manufacturing operativity.
In this contest, an example encountered during the development of GLP-1 analog processes will be described, showing the chemical solutions adopted to improve the physiochemical properties of critical raw materials and to ease the process operation [2,3].

[1] https://www.bioprocessintl.com/therapeutic-class/high-tides-lilly-s-20bn-spend-amgen-preps-network-to-enter-glp-1-space (accessed 20 January 2025)
[2] Patent pending
[3] Orlandin A. et al *Org. Process Res. Dev.* submitted

OC n° 11

PROCESS DEVELOPMENT AND OPTIMIZATION: A CASE STUDY ON TELESCOPIC DOUBLE SONOGASHIRA REACTIONS

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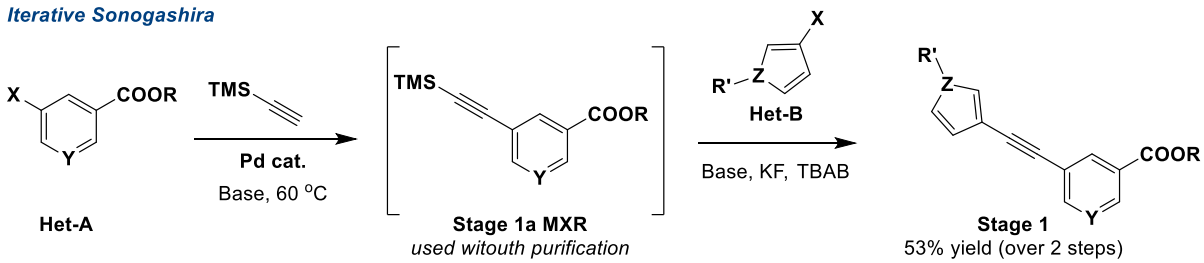
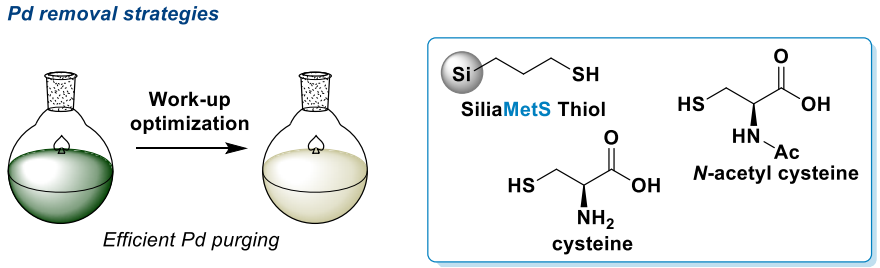
A case study focusing on two-step iterative Sonogashira cross-coupling process development and optimization is reported.
Palladium removal techniques were integrated into the process at intermediate stages to ensure compliance with stringent requirements for residual palladium content in the final product. These strategies combined washing techniques, adsorption methods and tailored crystallization steps to achieve substantial reductions in palladium residues.
Finally, an unforeseen issue arising from morphological differences in potassium fluoride (KF) from various raw material sources, which impacted the outcome of the Sonogashira cross-coupling reaction, was identified before process scale-up and addressed through root cause analysis and targeted solutions.





The lessons learned from this case study highlight the importance of balancing process efficiency with adherence to required standards in pharmaceutical manufacturing.

OC n° 12

PD-CATALYZED COUPLING OF 1-(2-(ALLYLOXY)PHENYL)-2-YN-1-OLS AND ISONITRILES FOR THE SYNTHESIS OF 2-(BENZOFURAN-2-YL)ACETAMIDES

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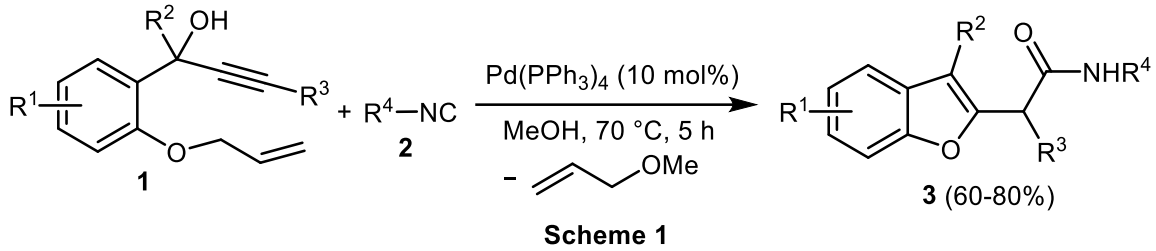
(2-(Benzofuran-2-yl)acetamides represent a class of organic compounds of particular interest, due to their significant pharmacological activities, including antifungal [1] and anticonvulsant [2,3] activities, in particular. Their structural versatility makes them promising candiPresents for drug discovery and development, motivating research efforts aimed at developing new methods for their synthesis as well as at understanding their biological functions and therapeutic potential.

In this contribution, a novel catalytic method is presented, which allows the synthesis of 2-(benzofuran-2-yl)acetamides **3** starting from readily available 1-(2-(allyloxy)phenyl)-2-yn-1-ols **1** and isonitriles **2** and with $Pd(PPh_3)_4$ as simple catalyst (Scheme 1). Reactions are carried out in MeOH at 70 °C for 5 h.



Scheme 1

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

[1] C. Mahecha-Mahecha, P. Borrego-Muñoz, L.M. Pombo, D. Gamba-Sánchez, *RSC Adv*. **2023**, *13*, 25296-25304.
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OC n° 13

RECYCLING OF RARE EARTH ELEMENTS: FROM E-WASTE TO STEREOSELECTIVE CATALYTIC REACTIONS

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Raw mixtures of Rare Earths Elements, REE, recovered by E-waste, were used as catalysts to promote the (stereoselective) synthesis of highly valuable compounds. Y_2O_3, the major species that is recovered by the E-waste, can be easily converted into the catalytically active $Y(OTf)_3$ that is able to efficiently promote the Michael addition of indoles to benzylidene malonates and the stereoselective Diels-Alder cycloaddition between cyclopentadiene and 4-(*S*)-3 acryloyl 4-tert-butyl 2-oxazolidinone.[1]
Additionally, the raw mixtures were immobilized onto silica [2] through a noncovalent interaction between $Y(OTf)_3$ and phosphotungstic acid (PTA) that is anchored onto amine-functionalized silica (Figure 1).

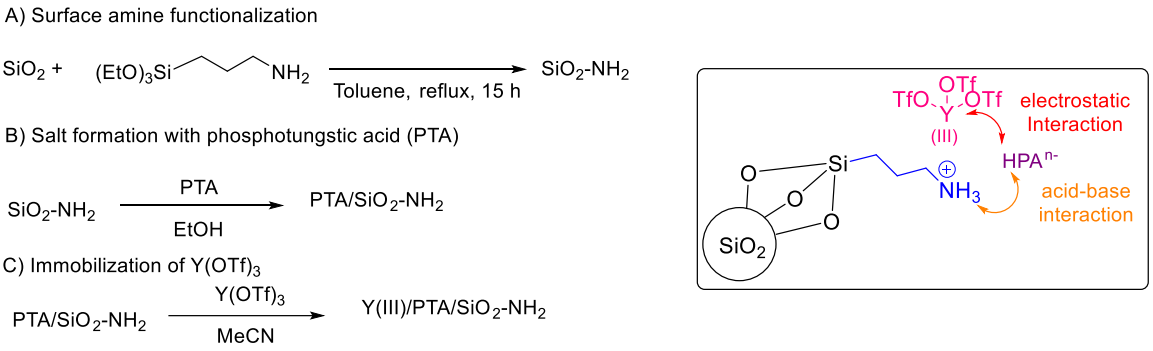

Figure 1.

The supported catalysts were used to construct packed-bed reactors,[3] resulting in values for Productivity and Space-Time Yields that were significantly higher than those of the corresponding batch conversions (Figure 2). Notably, the prepared cartridges maintained their catalytic efficiency over prolonged continuous operation.[4]

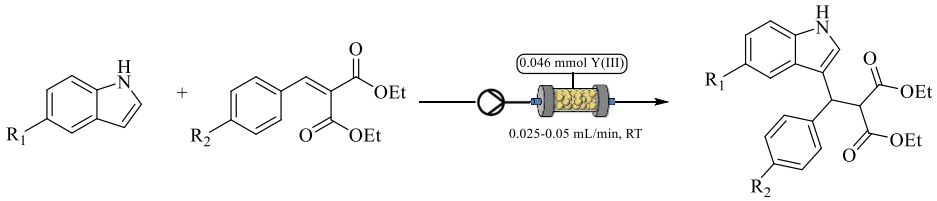

Figure 2.

[1] E. Donato, F. Medici, V. Chiroli, A. Puglisi, C. Rogoli, P. Fröhlich, M. Bertau, G. Zanoni, M. Benaglia, *ChemSusChem* **2024**, e202401787.
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OC n° 14

EXPANDING THE BOUNDARIES OF ORGANOCATALYSIS TOWARDS SUSTAINABILITY VIA ACID AND AMINOCATALYSIS

Fabio Pesciaioli,[a] Matteo Di Saverio,[a] Valeria Nori,[a] Giuliana Giorgianni,[a] Francesca Della Penna,[a] Emanuele Cocco,[a] Simone Mantegazza,[b] Gabriele Razzetti,[b] Giuseppe Quattrocchi,[b] Maria Edith Casacchia,[a] Pier Carlo Ricci,[c] Simone Di Muzio,[a] Andrea Lazzarini,[a] Stephen Thomas,[d] Pietro Allegrini,[e] Armando Carlone[a]

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In the last 20 years, organocatalysis became a valuable toolbox for constructing complex molecules or simply tackling synthetic problems at academic and industrial level, being considered a complementary platform to metal- and biocatalysis. Our research group constantly focuses on expanding the boundaries of organocatalysis trying on one hand to provide a solution to long standing problems of this scientific field and in the other to apply the mild and eco-friendly features of organocatalysis towards the synthesis of relevant pharmaceutical motifs. Industrial R&D routinely screens organocatalysis as a technology platform; however, its full applicability is sometimes hampered by the relatively high catalytic loading.
To address this issue, we developed a trivial immobilization strategy which allows to form simultaneously a bond between the catalyst and the support while generating the organocatalytic active site (Figure 1a).[1]

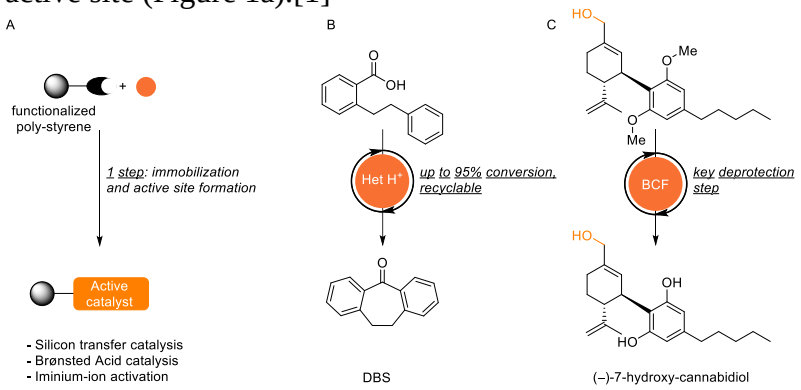

Figure 1. Suistanable approaches for catalysis and for the synthesis of valuable molecules.

Furthermore, exploiting the versatility of Brønsted and Lewis acid catalysis we reported the mild synthesis of Dibenzosuberone, employing Amberlyst-15 as heterogeneous catalyst [2] (Figure 1b), and 7-hydroxy-Cannabidiol relying on Lewis acid catalysed Piers-Rubinsztajn reaction in the key-step of the synthetic sequence [3] (Figure 1c).

[1] G. Giorgianni, M. Casacchia, P. Ricci, S. Di Muzio, A. Lazzarini, A. Carlone, F. Pesciaioli, *Synlett* **2024**, *35*. https://doi.org/10.1055/a-2349-1863; [2] V. Nori, F. Della Penna, E. Cocco, S. Mantegazza, G. Razzetti, G. Quattrocchi, F. Pesciaioli, A. Carlone, *ChemCatChem* **2023**, *15*, e202300642; [3] E. Cocco, D. Iapadre, A. Brusa, P. Allegrini, S. P. Thomas, F. Pesciaioli, A. Carlone *RSC Adv.* **2024**, *14*, 2741-2744.

OC n°15

HYDROXYPYRONE-BASED MATERIALS: DUAL FUNCTIONALITY FOR ANTIMICROBIAL IRON CHELATION AND WATER POLLUTANT DEGRADATION

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Hydroxypyrone-based (HPO) materials, derived from kojic acid, a natural metabolite of *Aspergillus species*, exhibit remarkable versatility for healthcare and environmental remediation [1]. Functionalized cryogels incorporating HPO and β-cyclodextrin serve as potent antimicrobial systems by chelating iron ions essential for bacterial survival. The β-cyclodextrin nanocontainers also enable controlled drug delivery, significantly enhancing bactericidal efficacy against Gram-positive and Gram-negative bacteria. These properties position hydroxypyrone-functionalized cryogels as promising candiPresents for advanced therapeutic applications, including wound dressings [2].

On the environmental front, hydroxypyrone-based porous polymers (C-HPO) exhibit exceptional chelation capacities for heavy metals, including mercury, copper, and iron [3]. When coordinated with iron ions, C-HPO forms a photo-Fenton-like system that generates reactive oxygen species (ROS) for pollutant degradation. This system effectively degrades emerging contaminants, such as antibiotics and industrial dyes, under mild conditions, achieving near-complete removal with minimal material usage.

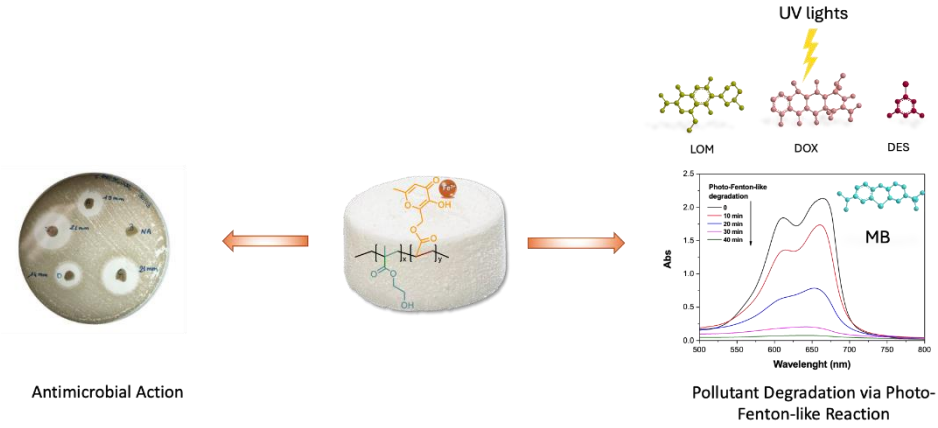

Figure 1. Illustration of C-HPO activities.

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OC n° 16

GLYCOCONJUGATED LUMINESCENT LANTHANIDE COMPLEXES AS DIAGNOSTIC PROBES

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Glycoconjugation is a powerful tool for imparting selectivity (Warburg effect) to therapeutic and molecular diagnostic agents, which, in the latter, is essential for an early detection of cancer.[1] Lanthanide-based probes possess peculiar photophysical properties in contrast to common organic fluorophores: their long luminescence lifetime allows time-resolved detection, an important advantage for bioassays and luminescence microscopy.[2] We have realized the glycoconjugation with different monosaccharides of a series of nine-coordinated neutral complexes (Eu(III) and Tb(III)) based on triazacyclononane, bearing dipicolinic acid-derived chromophoric ligand arms, the antenna, characterized by an electron-poor moiety (a pyridine ring) conjugated via a triple bond or directly to an electron-rich (para-substituted) phenyl ring (Figure 1).[3] This highly conjugated, rigid, and planar ligand system allows excellent sensitization of lanthanide ions with one or two-photon excitation processes. All complexes exhibited good photophysical properties (in line with the non glycoconjugated version), with excellent water solubility and stability. In addition, the Eu(III) complexes demonstrated the ability to stain the circulatory system of zebrafish embryos and to accumulate in xeno-grafted cancer cells.

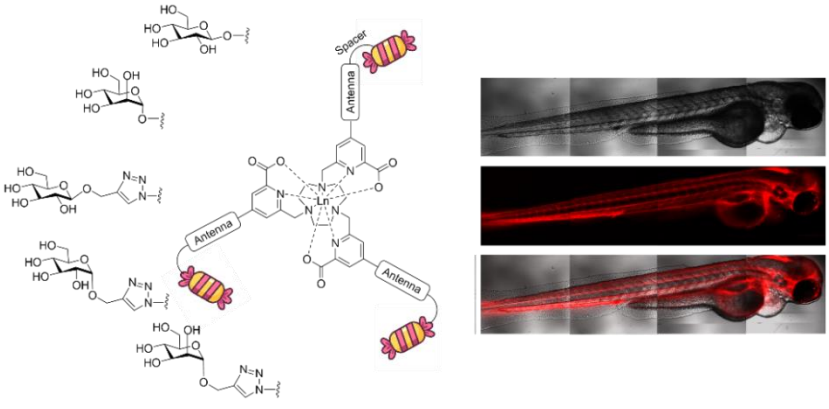

Figure 1.

[1] G. Bononi, D. Iacopini, G. Cicio, S. Di Pietro, C. Granchi, V. Di Bussolo, F. Minutolo, *ChemMedChem*, **2020**, *16*, 30-64.

[2] M. C. Santangelo, L. Lucchesi, L. Papa, A. Rossi, G. Egizzo, G. L. Fratello, L. Favero, M. Pineschi, V. Di Bussolo, S. Di Pietro, *Mini-Reviews in Medicinal Chemistry*, **2025**, *manuscript in press*.

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OC n° 17

A NEW, STRAIGHTFORWARD SYNTHESIS OF 3-DEOXY-3-AMINO D-GALACTOSE, A KEY STRUCURAL MOTIF OF GALECTIN LIGANDS

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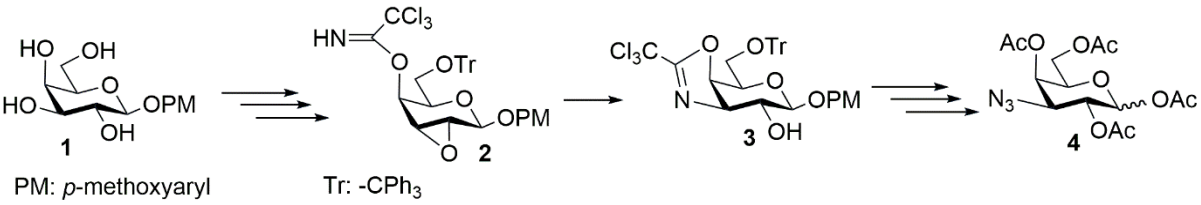
3-Amino-3-deoxy D-galactose and the 3-azido analogue became important targets in organic synthesis since the discovery that symmetrical sulfide or thioglycoside derivatives thereof, with an aromatic *N*-derivatization, can be excellent ligands of galectins. These latter are β-galactoside receptors playing a key role in multiple biological processes with relevant therapeutical implications [1], so that some inhibitors thereof reached clinical trial stages or even commercialization as drugs [2]. The most applied routes towards 3-amino (azido)-3-deoxy D-galactose are based on key S_N2 steps, aimed at setting the nitrogenated functionality with the right configuration [3-5]. In all the reported examples the main synthetic drawbacks (in terms of yield, cost, and experimental time) are invariably related to both the regioselective installation on the sugar scaffold of the suitable leaving groups, and the successful outcome of the subsequent S_N2 steps. We have recently designed a new synthetic strategy to convert galactose into 3-amino/azido-3-deoxy galactose derivatives relying on exclusive use of intramolecular S_N2 steps. The strategy was based on the generation of the key epoxide intermediate **2** (Scheme), bearing a trichloroacetimiPresent functionality at C-4 suitably oriented to carry out the nitrogen installation at C-3 via epoxide opening.



Scheme

In comparison with reported routes, this approach stands out in the sensible reduction of experimental times, the viable application of solvent-free conditions in four of the nine steps required, and a reduced number of chromatographical purifications of intermediates.

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OC n° 18

DESIGN AND SYNTHESIS OF A NEW TOLL LIKE RECEPTOR 4 AGONIST-BASED ANTIBODY DRUG CONJUGATE FOR CANCER IMMUNOTHERAPY

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TLR4 is an inflammatory Pattern Recognition Receptor (PRR), whose function is to sense Pathogens or Damages Associated Molecular Patterns (PAMPs, DAMPs) and start the innate immune response.[1] The natural ligand of TLR4 is Lipopolysaccharide (LPS), an essential component of Gram-negative bacteria outer membrane.[1], [2] The minimal portion of LPS required for immunogenicity is a glycolipid called Lipid A.[2] Through molecular simplification starting from Lipid A, our group developed a set of new compounds which showed promising TLR4 agonism: FP-20 (Fig.1, a) and the Glycosilated FP-20 serie.[3] Giovanna D'Amico's group showed that FP-20 and Rhamnosylated FP-20 (FP-20-Rha, Fig. 1, b) are able to shift macrophages' phenotype from carcinogenic M2 to anti-cancer M1. Activated macrophages are cytotoxic towards the leukemia 697 cell line.
Thus the compounds produced by our group can be used as payloads in an Antibody-Drug Conjugate (ADC) to be exploited in cancer immunotherapy.
The aim of this work is to conjugate FP-20 and FP-20-Rha to a linker suitable for the conjugation with several antibodies. At this purpose we selected the cathepsin cleavable linker Val-Cit-PAB-OH bearing a maleimidocaproic (MC) moiety (Fig.1, c). Conjugation with different antibodies will be carried on to test FP-20 and FP-20-Rha in therapy towards different cancer cell lines.

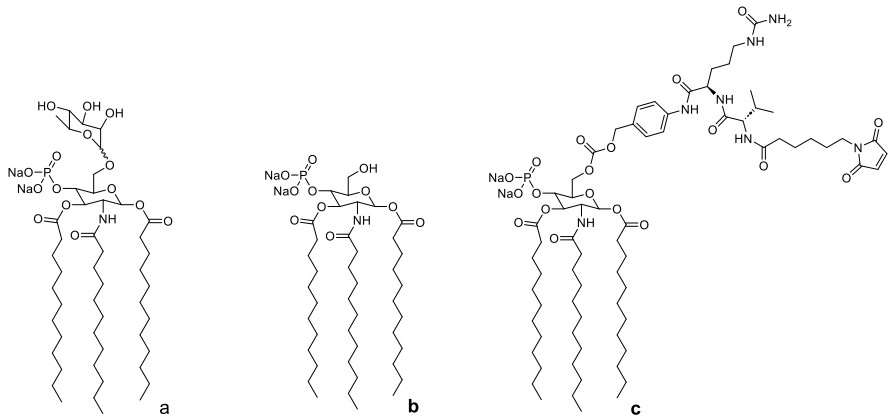

Figure 1. a) FP-20, **b)** FP-20-Rha, **c)** FP-20 conjugated to the MC-Val-Cit-PAB-OH linker.

[1] R. Medzhitov. Toll-like receptors and innate immunity. *Nature Reviews*, **2001**.
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[3] A. Romerio *et al.*, Overcoming challenges in chemical glycosylation to achieve innovative vaccine adjuvants possessing enhanced TLR4 activity *ACS Omega*, **2023**.

OC n° 19

CHIRAL MOLECULAR RECOGNITION BY PRISM[n]ARENES MACROCYCLES

Ernesto Santoro,[a,*] Paolo della Sala,[b] Carmine Gaeta,[b] Stefano Superchi[a]

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Chiral sensing has gained great interest in the recent years, due to its application in several fields, such as medicinal chemistry, environmental control, and natural products. Among the most promising molecular structures for chiral sensing and recognition are the so-called stereodynamic chiroptical probes [1]. To this family belong polyaromatic host macrocycles having planar chirality, able provide host-guest complexes with chiral guests in which the host exhibits a preferred chiral conformation that correlates with the absolute configuration (AC) of the guest. In 2020 a novel class of macrocyclic hosts named prism[n]arenes PrS[n]R (n = 5 and 6, in Fig. 1) have been reported by Gaeta and coworkers [2]. Prismarenes are constituted by 1,5-methylene bridged 2,6-dialkoxynaphthalene units and exhibit a deep π-electron rich aromatic cavity, thus being able to form endo-cavity complexes with ammonium guests stabilized by secondary interactions such as cation···π, C–H···π, van der Waals, and hydrophobic effect. For these macrocycles, the changes in the chiral conformations of the probe can be easily detected and interpreted by means of Electronic Circular Dichroism (ECD) spectroscopy due to its ability to discriminate between enantiomers [3]. In this work, we report the study of the chiral induction and host/guest interactions among different chiral guests and Prism[n]arenes hosts supported by ECD measurements and their DFT simulation.

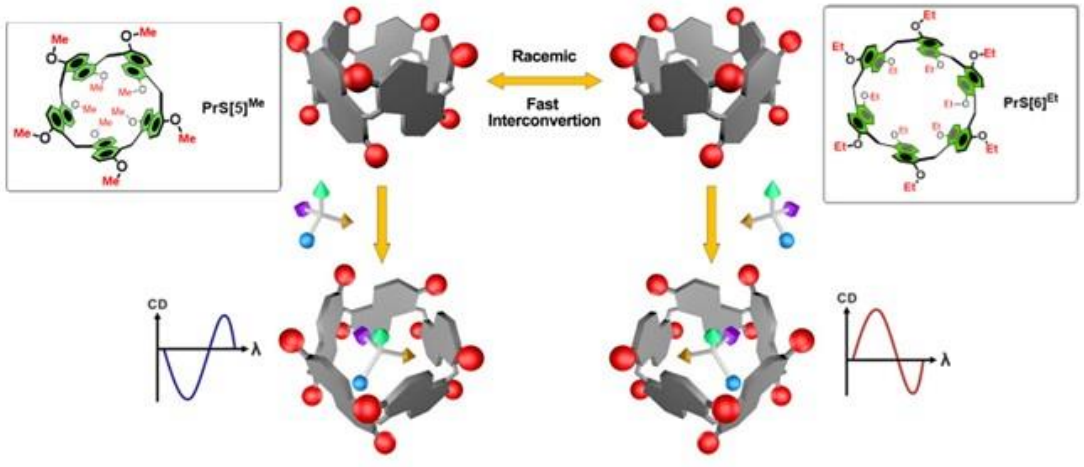

Figure 1.

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OC n° 20

A NOVEL PHOTOCATALYZED STRATEGY FOR THE TELESCOPIC SYNTHESIS OF SUBSTITUTED 1-PYRROLINES

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In this study, we present a mild synthetic protocol for producing nitrogen-containing five-membered rings, which serve as valuable intermediates for constructing numerous molecular structures commonly found in active compounds with anti-inflammatory, antiseptic, antibacterial, and anticancer activities [1].
This approach offers significant advantages due to the broad availability of starting materials, such as free amine and beta keto derivatives. Through the presented process these feedstocks can be easily and efficiently converted into complex N-heterocyclic structures through a straightforward two-step process (Figure 1).
The key step in this synthetic pathway is a metal-free photoredox-catalyzed reaction [2], which demonstrates excellent compatibility with a wide range of common functional groups. This method is also environmentally advantageous, offering ideal atom economy and eliminating the need for precious metal catalysts.

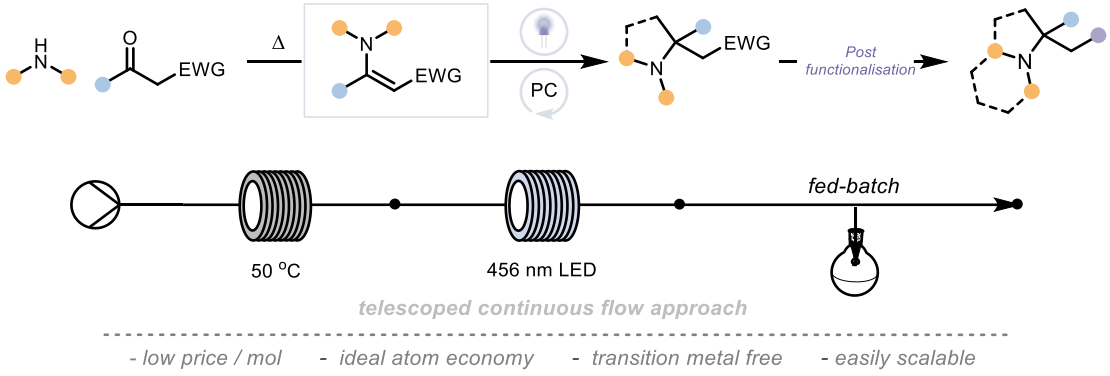

Figure 1.

Moreover, we assess that the second synthetic step can be sequentially conducted without purification. Indeed, the thermal process has been telescoped [3] with the photochemical step in which the photocatalyzed reaction is accelerated under intensified conditions of light irradiation [4].

Acknowledgment: we are grateful to have received funding from the (PlaDisPho) SOE_0000091 (PNRR).

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OC n° 21

OXIDATIVE ANIONIC HOMO-FRIES REARRANGEMENT UNDER BENCH-TYPE AEROBIC CONDITIONS

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The development of new protocols which enable the use of aerobic/protic conditions in alkali-metal-mediated transformations has reshaped the conceptual chemistry of these highly polar organometallic reagents. Our findings in this field disclosed that highly reactive alkyllithiums can efficiently promote chemoselective nucleophilic acyl substitution (S_NAc)[1] and regioselective metalation[2,3] reactions using deep eutectic solvents (DESs) or cyclopentyl methyl ether as sustainable reaction media, working at room temperature, in the presence of moisture and air. Recently, we also illustrated the usefulness of lithium amides to promote the chemo- and regioselective anionic Fries rearrangement of *O*-aryl carbamates under bench-type conditions.[4,5] As an extension of our methodology, we now exploit the use of aerobic conditions to induce the oxidation of benzylic anions generated from *O*-tolyl carbamates upon a metalation-*homo*-Fries rearrangement sequence in 2-MeTHF. Conversely, when protic DESs are used as reaction media only the rapid *homo*-Fries rearrangement occurs, and the oxidation step is efficiently suppressed owing to the competitive protonolysis of organolithiums.

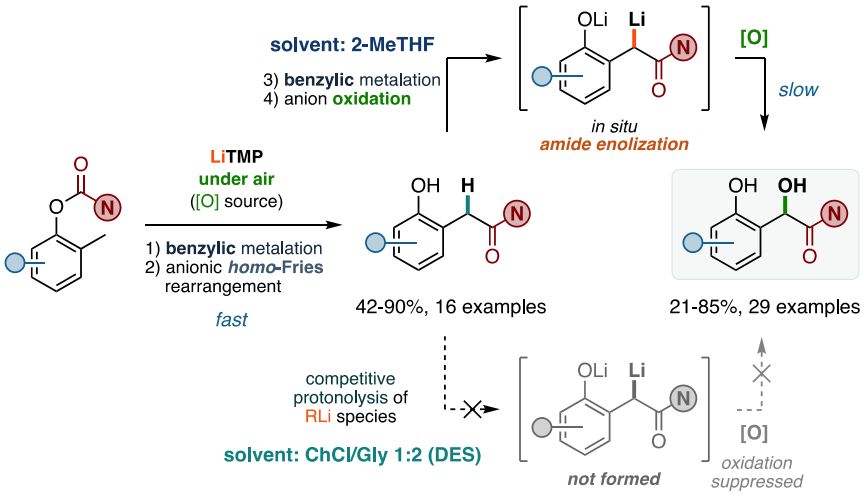

Figure 1.

This work was funded by "Unione Europea-Next Generation EU, Missione 4 Componente 1 CUP: D53D23010260006".

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OC n° 22

FLUORINATED CLIMACOSTOL, A NEW POTENTIAL SMALL MOLECULE CANCER CHEMOTHERAPEUTIC AGENT

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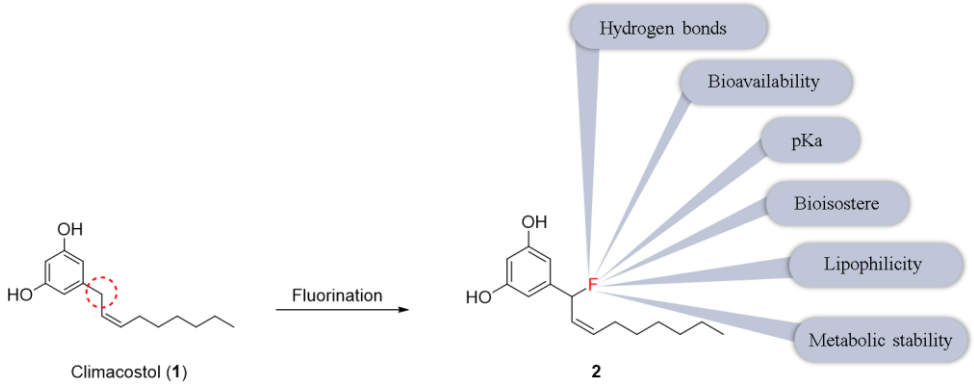
The use of fluorine in chemistry is expanding fast, due to its exclusive properties and to the benefits of its introduction into molecules with biological activity. In fact, the introduction of fluorine changes the properties of biological molecules, such as pKa, lipophilicity and metabolic stability. Organofluoride compounds are substrate mimetics of the corresponding nonfluorinated compounds in enzymatic reactions in fact the C-F bond is a bioisostere of either C-O or C-H, where most enzymes do not discriminate the C-F bonds form the corresponding C-H or C-O bonds [1-3].
Based on these considerations and given the experience of our group in the synthesis of analogues of climacostol (**1**), a natural resorcinolic lipid that, in addition to its physiological functions, shows biological activities indicating it to be an effective antimicrobial and anticancer agent [4], we decided to develop the synthesis of a new fluorinated analogue (**2**). After several attempts with the most recent fluorination methodologies [5], our target fluorinated small molecule was obtained using DAST, a powerful reagent utilized for the conversion of alcohols into corresponding fluorides. The optimization of the synthetic methodology of 2 will allow to verify whether it is ideal candiPresent for cancer research, i.e. to be able to exhibit cytoprotective properties against normal cellos and cytotoxic effects on malignant cells.



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OC n° 23

SEQUENTIAL INSERTION OF CARBON MONOXIDE AND CARBON DIOXIDE FOR THE SYNTHESIS OF BENZOXAZINONE DERIVATIVES

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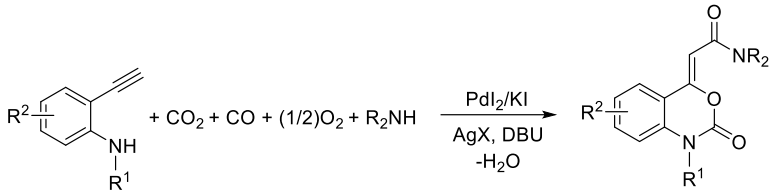
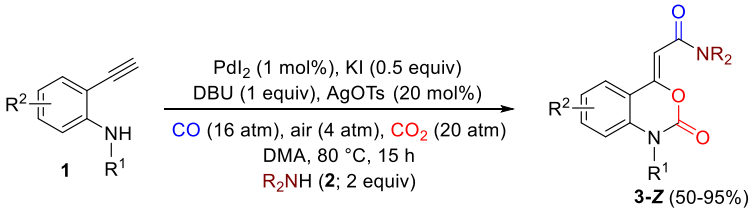
1,4-Dihydro-2*H*-benzo[*d*][1,3]oxazin-2-ones are an important class of heterocyclic derivatives, which display a wide range of applications in medicinal chemistry.[1] For this reason, the synthesis of differently functionalized 1,4-dihydro-2*H*-benzo[*d*][1,3]oxazin-2-ones has attracted considerable attention in recent years.[2,3]

In this communication, we report an innovative approach to dialkyl-2-(2-oxo-1,2-dihydro-4*H*-benzo[*d*][1,3]oxazin-4-ylidene)acetamides through the catalytic multicomponent assembly of several simple units, namely, 2-ethynylanilines, carbon monoxide, and carbon dioxide, and secondary amines. The new synthetic process consists in a PdI_2-catalyzed oxidative monoaminocarbonylation[4] of the triple bond of 2-ethynylanilines followed in situ by DBU/Ag^+-promoted carbon dioxide insertion with 6-*exo*-*dig* cyclization (Scheme 1).



Scheme 1. Synthesis of dialkyl-2-(2-oxo-1,2-dihydro-4*H*-benzo[*d*][1,3]oxazin-4-ylidene)acetamides by sequential insertion of carbon monoxide and carbon dioxide into 2-ethynylanilines

Reactions are carried out using 1 mol% of PdI_2 and 0.5 equiv of KI, in DMA as the solvent, at 80 °C and under 40 atm of a 4:1 CO-air mixture and 20 atm from CO_2, in the presence of 2 equiv of a secondary amine **2**, with 1 equiv of DBU and 0.2 equiv of AgOTs. The value high added 1,4-dihydro-2*H*-benzo[*d*][1,3]oxazine derivatives **3** are formed in good to high isolated yields (50–95%) starting from variously substituted substrates (Scheme 2). The structure of a representative product, including the *Z* stereochemistry around the exocyclic double bond, has been confirmed by XRD analysis.



Scheme 2

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OC n° 24

REACTIVITY INSIGHTS OF ARYLBORONIC ACIDS IN *IPSO*-SUBSTITUTION REACTIONS

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Notably, recent advancements in borylation methods have made arylboronic acids readily accessible and widely utilized as versatile building blocks in organic synthetic transformations. These substances exhibit unique reactivity, enabling various carbon-carbon coupling reactions, such as the well-known Suzuki coupling, as well as carbon-heteroatom bond formations utilizing transition metal complexes [1]. These transformations encompass the introduction of oxygen, nitrogen, halogens, as well as alkyl, alkynyl, alkenyl, aryl and formyl moieties [2]. *Ipso* functionalization of boronic acids offered a site-specific substitution approach, effectively addressing the challenges of regio- and chemoselectivity that arise from traditional electrophilic substitution. This study enhances our understanding of the reactivity of arylboronic acids and highlights their versatility in synthetic applications.

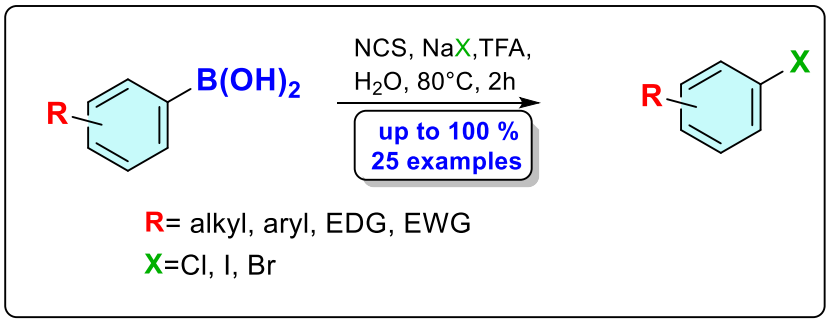

Figure 1. *Ipso*-functionalization of arylboronic acids

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OC n° 25

NEW SYNTHETIC METHODOLOGIES FOR THE CHEMO- AND STEREOSELECTIVE TRANSFORMATION OF SUBSTITUTED CYCLOBUTANES

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Continuing with our interest in exploring new reactivities of cyclobutanone derivatives, recently we studied the reactivity of α-hydroxy cyclobutanones with stabilized phosphonium ylides leading to the synthesis of functionalized cyclopropane carbaldehyde and 2-hydroxycyclobutylidene derivatives.[1] Building upon this strategy, further useful transformations were developed to construct diverse functionalized cyclobuta-fused-heterocycles[2], [3] and 4-substituted γ-lactones.[4] A new cascade reaction has been also discovered for efficient access to diverse structurally valuable 2-oxabicyclo [3.2.0] heptan-3-ones bearing a pendant benzo[d]oxazol-2(3H)-one moiety at the bridgehead quaternary center in moderate to good yields.[5]

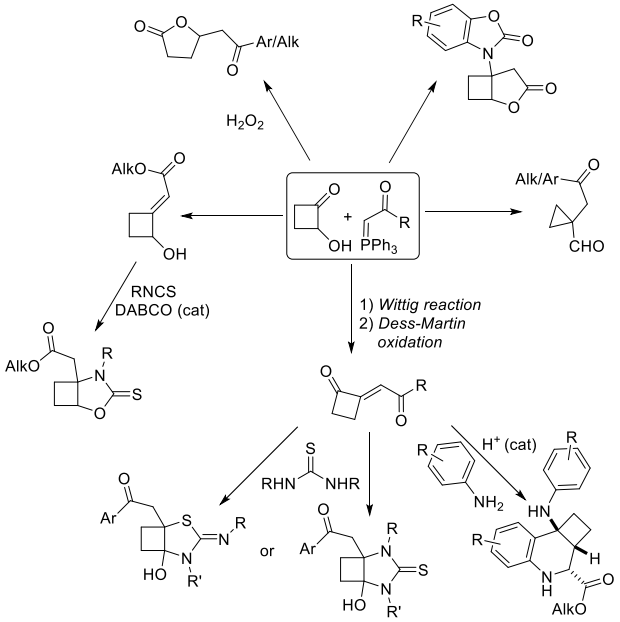

Figure 1.

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[5] Unpublished results

Flash Presentations

FP n° 1

MIRROR-IMAGE IMINOSUGARS: MULTIPOTENT GLYCOMIMETICS FOR THE TREATMENT OF RARE DISEASES

Anna Esposito,[a,*] Maria Stabile,[b] Valeria De Pasquale,[c] Luigi Michele Pavone,[b] Pedro Merino,[c] Atsushi Kato, [e] Eliana De Gregorio,[b] Annalisa Guaragna[a]

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Over the last few years, L-iminosugars, mirror images of the natural D-iminosugars, have shown promising pharmacological properties acting as selective inhibitors and/or enhancers of carbohydrate-processing enzymes involved in key biological functions [1]. However, these unnatural glycomimetics have been less explored compared to their D-counterparts as they are not available from natural sources and few routes have been developed for their chemical synthesis. Our attention has been focused on the preparation of L-*gluco* configured iminosugar L-DNJ and its alkyl/acyl derivatives (**Figure 1**) to evaluate their pharmacological properties.

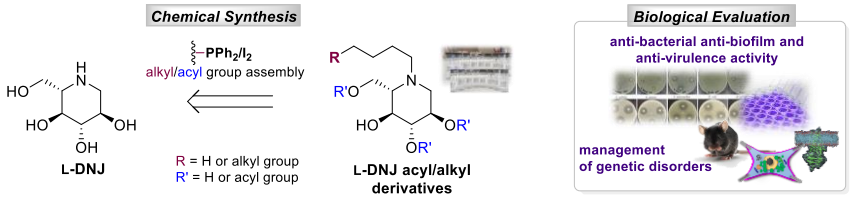

Figure 1. L-DNJ and its alkylated/acylated derivatives: synthesis and therapeutic applications.

Herein we report the synthesis of the pure L-DNJ, achieved by two novel procedures tuned up in our labs. With L-DNJ in hand, the established PS-TPP/I_2 activating system was exploited for both the assembly of the alkyl/acyl groups and their conjugation with iminosugar core giving access to a small library of L-DNJ derivatives. *In vitro* and *in vivo* assays revealed the potential of the synthesized compound in the treatment of genetic disorders, including Cystic Fibrosis [2], Pompe [3] and Mucopolysaccharidosis [4] diseases, as well as their antibacterial properties [5] pointing out their value of as novel promising broad-spectrum pharmacological tools.

The study was supported by a financial grant from European Cystic Fibrosis Society (ECFS) and Cystic Fibrosis (CF) Europe to A.E, by Italian Cystic Fibrosis Research Foundation (FFC), (#13/2020 and #8/2024) and by funds from the Cure Sanfilippo Foundation USA

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FP n° 2

EXPLORING HEPTACYCLIC LIGANDS: HOW OLIGO-HETEROARYLS INTERACT WITH G-QUADRUPLEX MOTIFS

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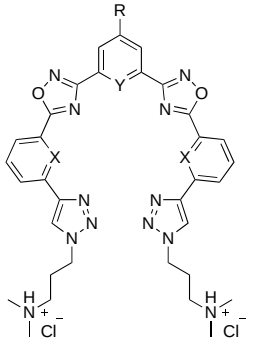
In the field of gene therapies, G-quadruplexes (G4s) are emerging as promising targets for treating several diseases, particularly in anticancer, antibacterial, and antiviral therapies. These non-canonical DNA and RNA secondary structures form in guanine-rich single-stranded sequences. [1] These structures assemble via π-stacking interactions, forming the stable G4 backbone. Stabilizing G4s represents a compelling strategy for therapeutic intervention. [2] We report the design, synthesis, and biophysical characterization of a novel family of water-soluble heptacyclic oligo-heteroaryls, developed to enhance selectivity and stabilization of G4 structures. These compounds feature a flexible oligoaryl scaffold containing N- and O-based heterocycles (Figure 1). The synthetic approach emphasizes modularity and efficiency, enabling structural diversification. Key innovations include the use of CuAAC chemistry for rapid and high-yield functionalization. The synthesized heptacyclic compounds demonstrated excellent water solubility under physiological conditions, largely due to the incorporation of tertiary amine side chains. Structural modifications allowed for an in-depth exploration of the role of pyridine versus benzene substitutions. Biophysical analyses, including FRET-melting and mass spectrometry, confirmed strong and selective G4 binding with minimal interaction with duplex DNA. Additional studies, such as Fluorescence Intercalator Displacement (FID) and molecular docking, suggested a mixed binding mode, where ligands interact within G4 grooves and end tetrads. This research highlights the potential of water-soluble heptacyclic oligo-heteroaryls as adaptable scaffolds for G4-targeting, enabling further functionalization for advanced molecular probes and therapies.



8	R=H	X=N	Y=N
14	R=H	X=CH	Y=N
15	R=H	X=N	Y=CH
16	R=H	X=H	Y=CH
21	$R=NO_2$	X=N	Y=N
22	$R=NO_2$	X=CH	Y=N
23	$R=NH_2$	X=N	Y=N
24	$R=NH_2$	X=CH	Y=N

Figure 1. Chemical structure of heptacyclic oligo-heteroaryls compounds.

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FP n° 3

FROM MICELLAR CATALYSED HYDROFORMYLATION AND HYDROAMINOMETHYLATION TO SOLID WASTE-BASED SUSTAINABLE PROCESSES

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Hydroformylation reaction is the most applied catalytic process in industry worldwide, being an efficient atom-economic reaction for the synthesis of linear aldehydes from olefines [1]. We have recently reported sustainable and generally appliable protocols for the regioselective hydroformylation [2] and hydroaminomethylation (HAM) [3,4] of terminal alkenes in water, taking advantage from both micellar and microwave catalysis. Moving from Green Chemistry [5] to Circular chemistry [6], a more sustainable solution has been proposed by replacing PEG-based surfactants with solid waste materials (SWMs). We report here a bio-based methodology for the hydroformylation in water of terminal olefins, using Sardinian White Wool (SWW) as waste-derived biomass, obtained as powder using mechanochemistry [7], as an additive to regioselectively produce valuable linear aldehydes. In a circular economy approach, SWW can be valorized, otherwise treated as special waste. The process is generally applicable to various terminal alkenes producing a library of linear aldehydes. The catalyst, the ligand, together with the biomass and H_2O, can be recovered and reused without a reliable decrease in conversion into the desired product and without using organic solvents, further reducing the environmental impact of the proposed methodology. Life Cycle Assessment (LCA) analyses confirm the efficiency and sustainability of this approach by comparing the new protocol with traditional hydroformylation methods. This proof of concept demonstrates the potential for SWMs to be used in the development of low impact catalytic processes, promoting a zero-waste approach.

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FP n°4

SYNTHESIS OF 1,2,3-TRIAZOLES IN THE GREEN SOLVENT CYRENE

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1,2,3-Triazoles are considered privileged scaffolds due to their diverse biological activities, sparking significant interest in the development of efficient and rapid synthetic methodologies [1]. Among these, the copper-catalyzed azide-alkyne cycloaddition (CuAAC) reaction is recognized as the most effective approach, widely applied in click chemistry for the joining of small molecular building blocks [2]. Solvents play a pivotal role in CuAAC by solubilizing the reaction components, namely azides, alkynes, and the Cu(I) catalyst formed in situ from a Cu(II) salt and a reducing agent. Conventionally used solvents such as dimethyl sulfoxide (DMSO), *N*,*N*-dimethylformamide (DMF), and tetrahydrofuran (THF), however, present significant drawbacks: DMSO and DMF are reprotoxic (H360) and THF is flammable and prone to forming hazardous peroxides [3].

We report a novel and sustainable protocol employing Cyrene, a biodegradable and non-toxic solvent, for the synthesis of 1,2,3-triazoles (Figure 1). This method circumvents the use of toxic solvents and offers significant operational advantages, including product isolation by simple precipitation in water, eliminating organic solvent extractions and chromatographic steps. This protocol not only reduces waste generation, but also lowers operational costs, allowing the reaction to be carried out on grams-scale. Its broad applicability is demonstrated with complex substrates, such as biologically active coumarins and triazole-linked bifunctional molecules. Additionally, the protocol is amenable to a one-pot, three-component reaction involving organic halides, terminal alkynes, and sodium azide, bypassing the isolation of organic azides, which are unstable intermediates with environmental sensitivity. This sustainable approach establishes a versatile and efficient pathway for triazole synthesis, aligning with green chemistry principles.

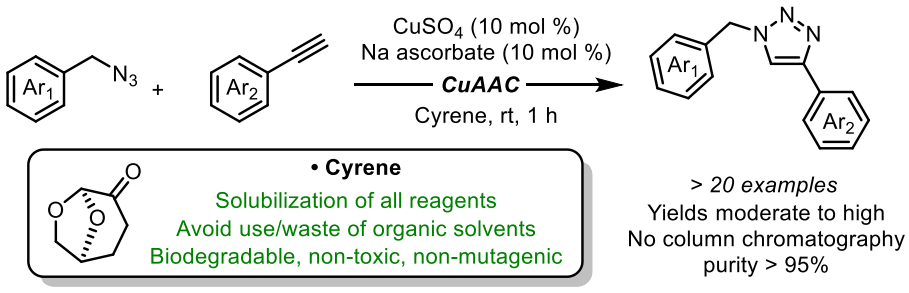

Figure 1. CuAAC reaction performed in Cyrene.

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FP n° 5

SYNTHESIS OF HERBOXIDIENE DERIVATIVES AS SPLICING MODULATORS

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Herboxidiene is a natural product known for its ability to modulate splicing by inhibiting spliceosome function. Like other small molecules, it interacts with SF3B1 subunit of the spliceosome, offering a selective therapeutic strategy. Indeed, it exhibits antitumor and antimicrobial properties, making it a subject of interest in drug discovery [1,2]. This study explores novel splicing modulators, particularly C6- and C12-modified herboxidiene derivatives, and introduces an efficient approach for their total synthesis. We present a stereodivergent strategy (retrosynthetic pathway in Scheme 1) in which two fragments, C1-C9 (**2a-c**) and C10-C19 (**3a-c**), are synthesized separately and combined in the final step using a Suzuki cross-coupling.

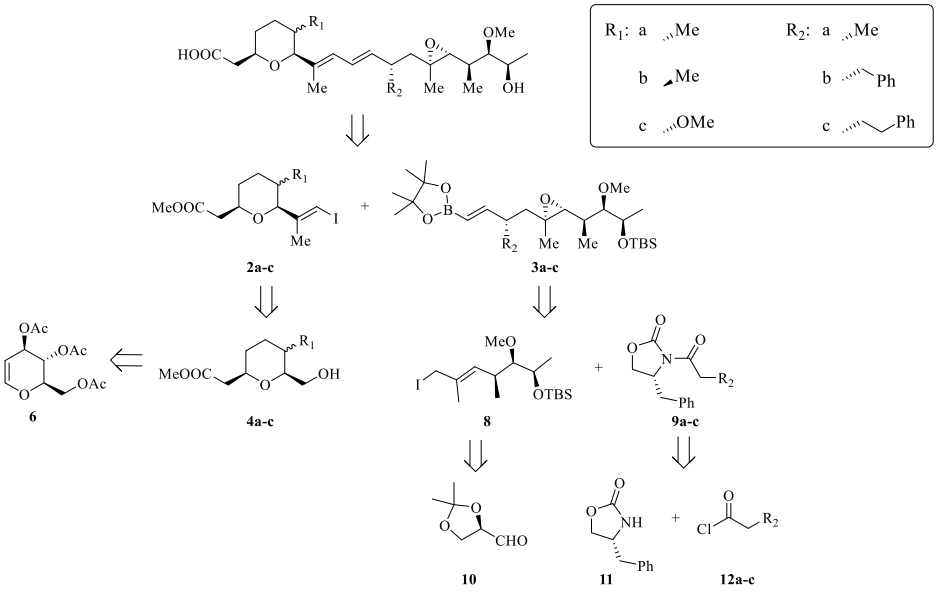

Figure 1. Retrosynthetic analysis proposed for the synthesis of herboxidiene derivatives.

Fragment C1-C9 is obtained from compound **6**, an excellent starting material already utilized by Gosh et al. [3], using a newly proposed 11-step protocol that allows the introduction of the C6-modifications. Fragment C10-C19 is prepared according to a previously reported procedure [4], introducing different Evans' chiral auxiliary to include the C12-modifications. This study presents preliminary results for the synthesis of compound **2a** and **2b** and of N-acyloxazolidin-2-one **9a-c**, highlighting the feasibility of this approach.

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FP n° 6

MILD-TEMPERATURE HYDROSILYLATION FOR EFFICIENT FUNCTIONALIZATION OF A POROUS SILICON BIOSENSOR FOR TROPONIN DETECTION DURING MYOCARDIAL INFARCTION

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Cardiovascular diseases (CVDs), particularly myocardial infarction (MI), are the leading cause of death in developed countries, with significant economic and healthcare costs. Early detection of MI is crucial for preventing irreversible damage, and cardiac troponin T (cTnT) is one of the most reliable biomarkers for diagnosing this condition.[1] Porous Silicon (PSi) has emerged as a promising material for biosensor development due to its unique properties, including surface tunability and high sensitivity. Nevertheless, effective functionalization of PSi surfaces remains a challenge. In this frame, we studied and set up a one-pot synthetic strategy for the functionalization of PSi that simultaneously stabilizes and decorates its surface with a shortened peptide nucleic acid through hydrosilylation chemistry. Combining mild temperatures and a Lewis acid catalyst, we have significantly reduced both the prolonged reaction times and high temperatures typically associated with conventional hydrosilylation.[2]

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FP n° 7

DESIGN AND SYNTHESIS OF POLYAMINES TO DEVELOP HIGHLY PERFORMING FERRITIN-CONJUGATES

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Cancer is a major global health and socioeconomic challenge. Although significant progress has been made and various drugs are available for treatment, the development of resistance remains a critical limitation, often leading to treatment failure.[1] Recently, novel therapies exploiting small interfering RNA (siRNA), micro-RNA mimics (miR mimics), and antisense micro-RNA (antagomiR) have been extensively explored for the treatment of cancer, neurodegenerative, and rare diseases.[2] Over the past decade, to overcome the challenges posed by delivery systems like nanoparticles made of potentially toxic exogenous materials, promising strategies have emerged. These include the use of protein-based platforms (HumAfFt) and chemical modifications of traditional oligoribonucleotides to enhance RNA delivery, stability, and efficacy.[3] Encapsulation of RNA in HumAfFt relies on polycationic molecules (PCs), which bind specifically to the protein and stabilize oligonucleotides via electrostatic interactions. To explore structure-encapsulation relationships between PCs and oligonucleotides, a library of polyamine molecules (PA) (Figure 1) was rationally designed and synthesized, incorporating a pentafluorobenzene sulfonamide moiety to anchor the polyamines to the cysteine residues of HumAfFt. The first series, featuring cyclic amines, was synthesized through successive reductive amination reactions starting from N-methyl-4-piperidone, with a final step introducing the pentafluorobenzene group. Conversely, linear PAs were prepared using Steglich couplings to combine glycine, β-alanine, and methylamine as key building blocks, followed by selective thiol-reactive group introduction. Cyclic PAs demonstrated efficient siRNA delivery and effective silencing of glyceraldehyde-3-phosphate dehydrogenase (GAPDH) gene expression across three cancer cell lines.

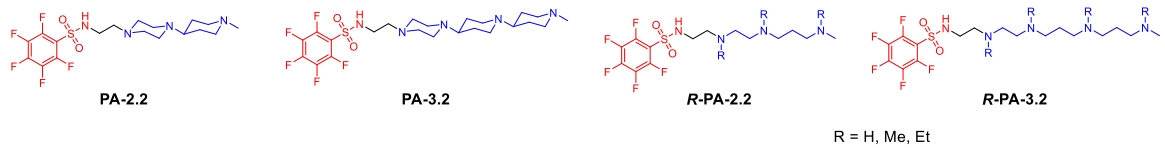

Figure 1. Chemical structures of polyamine molecules **PA-2.2**, **PA-3.2**, ***R*-PA-2.2**, and ***R*-PA-3.2**.

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FP n°8

SEMI-SYNTHETIC PATHWAYS TO OBTAIN GLYCOSAMINOGLYCANS MIMETICS FROM SUSTAINABLE SOURCES

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Sulfated glycosaminoglycans (GAGs) are highly complex, anionic, linear polysaccharides extracted from extracellular matrix of animals cells. Some of them are exploited in already approved therapeutic treatments, and a significant number of novel drugs are currently under development [1]. Nonetheless, naturally occurring GAGs exhibit variable chemical compositions and biological activities, which could cause unpredictable results during applications (*e.g.* heparin crisis in 2007). However, sulfated polysaccharides can also be obtained in a semi-synthetic way: the introduction of sulfate groups into the backbones of natural unsulfated polysaccharides allows to endow them with bioactivities similar to sulfated GAGs but without risks derived from their typical animal sources [2]. This work is focused on the development of semi-synthetic strategies for the regioselective modification of polysaccharides to obtain new polysaccharide-based products, which can be proposed as substitutes for GAG-based drugs already existing but obtained from less eco-sustainable sources.

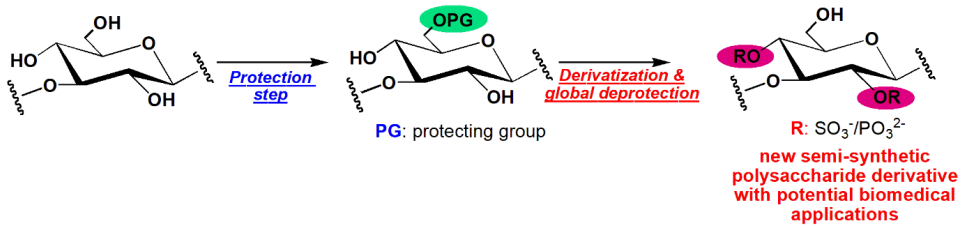

Figure 1.

The regioselective derivatizations that are carried out aim at the insertion of negatively charged functionalities (sulfate or phosphate groups), in order to mimic the structural characteristics of natural GAGs. The starting materials are polysaccharides extracted from bacterial or algal sources. In particular, the attention is focused on the development of suitable multi-step sequences all relying upon protection-derivatization-deprotection sequences [3,4].

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FP n° 9

CARBENOID-LIKE STRATEGIES FOR EXPANDING THE CHEMICAL SPACE OF HALOGEN-CONTAINING MANIFOLDS

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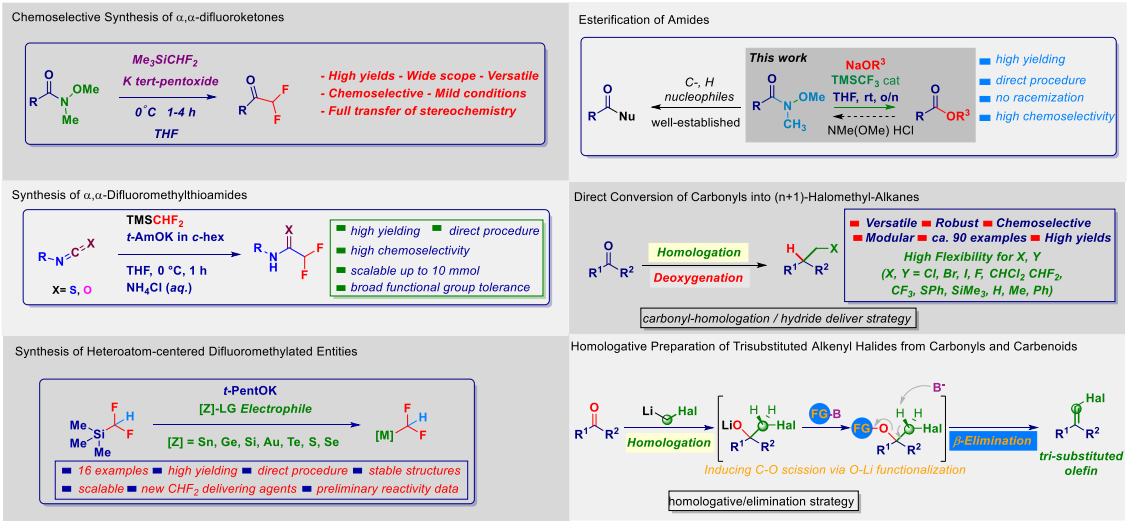
In recent years, carbenoid-based chemistry contributed to the development of novel homologating methodologies enabling the access to a variety of functionalized carbon arrays of progressive molecular complexity. Among the portfolio of nowadays available carbenoid-type homologating agents, those ones embodying one or more fluorine atoms manifest a higher tendency to decompose, making particularly challenging the innate synthetic potential. The use of the bench-stable $TMSCHF_2$, as pro-nucleophile (under alkoxide-activation) for delivering the valuable CHF_2 group, allowed the access to difluoromethyl ketones (from Weinreb amides) [1], difluoro(thio)amides [from iso(thio)cyanates] [2] and to various difluoromethyl-metal species (from electrophilic metals) [3]. Interestingly, the analogous Ruppert-Prakash reagent - acting as a versatile catalyst - allowed the intuitive, rather challenging, conversion of Weinreb amides into esters *via* the straightforward treatment with alkoxides [4]. The sequential homologation/hydride transfer into a carbonyl, furnishing halomethyl alkyl derivatives [5], alternatively the sequential homologation/E2-type elimination triggered on the tetrahedral intermediate with thionyl chloride furnished trisubstituted alkenyl halides starting from ketones and aldehydes [6].



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FP n° 10

SUSTAINABLE BIOPOLYMERIC CATALYTIC SYSTEM FOR *SUZUKI-MIYAURA* REACTIONS IN AQUEOUS MEDIA

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The *Suzuki-Miyaura* reaction is a cornerstone of organic synthesis and is widely recognized for its efficiency in constructing biaryl compounds (Figure 1). It is particularly valued for its mild conditions and broad functional group tolerance [1]. However, conventional homogeneous palladium (Pd) catalysts present significant sustainability challenges, including Pd leaching and reliance on toxic solvents. To address these limitations, we developed a sustainable biopolymeric catalyst (C-PhebPd) synthesized via radical polymerization of phenylalanine, modified and complexed with Pd ions, under subzero temperatures [2,3]. Comprehensive characterization by SEM, FTIR, and XPS revealed that this eco-friendly catalyst exhibits high porosity, excellent stability, and superior catalytic performance in water-based solvents [4]. C-PhebPd achieved quantitative yields across various substrates in *Suzuki-Miyaura* reactions, maintaining consistent efficiency over multiple catalytic cycles. Its fast reaction kinetics, recyclability, and reduced environmental impact position it as a promising, sustainable alternative for catalytic applications in organic synthesis.

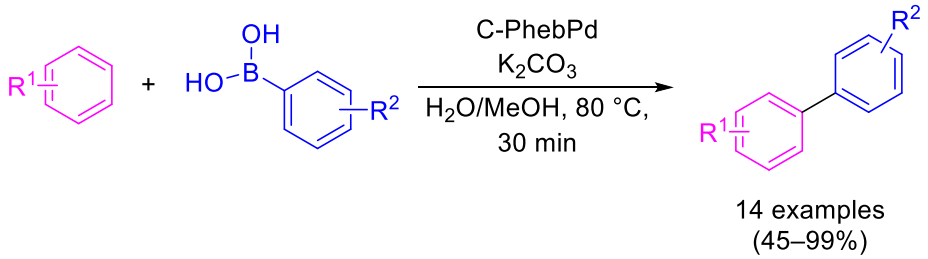

Figure 1. General scheme of *Suzuki-Miyaura* reactions catalyzed by C-PhebPd.

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FP n° 11

EMBRACING A NEW FRONTIER: MASTERING NICKEL-CATALYZED CROSS-ELECTROPHILE COUPLING REACTIONS IN DEEP EUTECTIC SOLVENTS

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Nickel-catalyzed cross-electrophile coupling reactions provide a compelling alternative to traditional coupling methods, significantly reducing the dependence on sensitive and expensive organometallic reagents [1]. In recent years, the use of sustainable solvents, such as Deep Eutectic Solvents (DESs) and water, has gained momentum in organometallic chemistry [2,3]. Building on our interest in developing sustainable catalytic cross-coupling reactions under aerobic conditions [4,5], we report here a groundbreaking nickel-catalyzed cross-electrophile coupling (XEC) reaction performed in environmentally benign DESs. This work marks a significant advance in green synthetic methodologies, combining the benefits of sustainable solvents with the exceptional activity of nickel catalysts. The developed system enables the direct coupling of electrophiles species, such as aryl halides and alkyl halides, under mild reaction conditions, achieving good yields and selectivity without requiring expensive metals or hazardous reagents (Fig. 1). Our findings not only underscore the feasibility of integrating DES with nickel catalysis, but also pave the way for exploring DESs in other complex catalytic processes, offering new perspectives for sustainable ed efficient synthetic strategies.

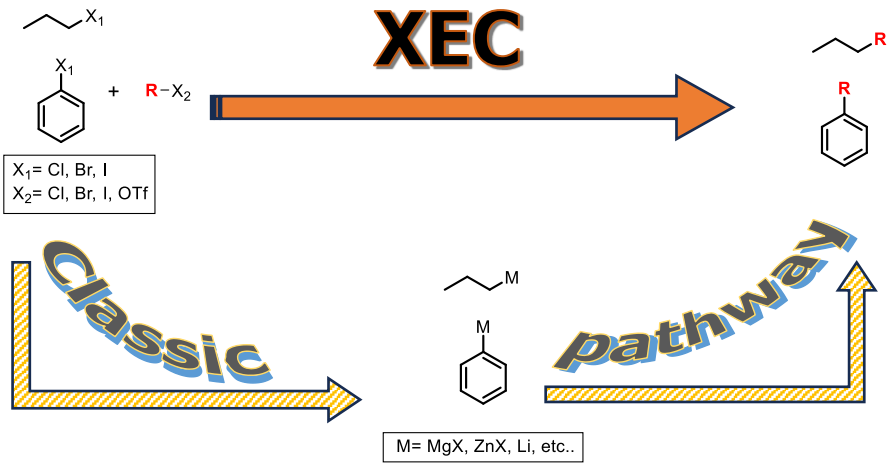

Figure 1.

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FP n° 12

MECHANOCHEMICAL SYNTHESIS OF SECONDARY AMINES VIA BORROWING HYDROGEN STRATEGY

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Amines are crucial in pharmaceuticals and fine chemicals, acting as intermediates in drug synthesis and materials.[1] *N*-alkylated amines are vital due to their role in bioactive molecules like benzonatate and bumetanide [2]. Traditional synthesis methods using alkylating agents pose risks such as overalkylation and genotoxicity, prompting the search for safer alternatives. Alcohols, with their abundance and low toxicity, are promising but limited by poor electrophilicity. The borrowing hydrogen (BH) strategy offers a green solution, using alcohols for amine alkylation through catalytic processes, reducing waste and simplifying purification.[3] Typically, Ru catalysts facilitate this process, producing water as the sole by-product. However, industrial use faces challenges like high catalyst loadings and harsh conditions.

Mechanochemistry, especially with ball milling, presents a sustainable alternative to traditional synthesis, avoiding or reducing use of solvents, enhancing catalyst efficiency and broadening synthetic applications [4,5]. Integrating mechanocatalysis with BH strategies addresses traditional limitations, offering a greener pathway for *N*-alkylation of amines. This communication will explore the mechanochemical *N*-alkylation of amines via Ru-catalyzed BH, highlighting advancements, challenges, and the potential of this methodology to drive sustainable chemical manufacturing.

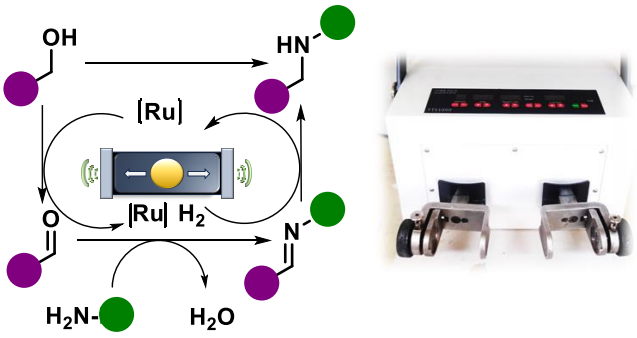

Figure 1. Mechanochemical BH.

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FP n° 13

IN SILICO DESIGN OF NEW ANTIBACTERIAL DRUGS AND LIGAND-PROTEIN INTERACTION STUDIES TARGETING COX-1

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The design of new drugs is a fundamental aspect of the pharmaceutical industry. Expanding the therapeutic spectrum of existing bioactive molecules and developing new therapies are the primary objectives of pharmaceutical research. In recent years, the study of COX-1 has gained significant attention, especially with the discovery of its overexpression in certain human pathologies [1]. Designing new compounds is challenging and time-consuming, as identifying modifications to enhance ligand-protein interactions is often difficult, leading to significant waste of time and resources in laboratories. Molecular Docking could be the solution, because it is an effective and competent tool for in silico screening that permits us to evaluate at the same time a lot of compounds. Using a comprehensive online database of readily available bioactive compounds, we identified molecules like four template compounds, that is COX-1 inhibitors from the diarylheterocycle class, renowned for their significant biological and antibacterial activities [2]. These compounds were then imported into the FLAP software. It identifies interaction fields (MIFs), computed in GRID [3], and operates in a structure-based virtual screening (SBVS) mode, studying interactions between the molecules being analysed and the calculated protein pockets [3]. These virtual screenings can be excellent starting points for the construction of a large database of compounds. Additionally, a parallel line of research concerning green pistachios has enriched this project by providing a diverse source of bioactive compounds. Many of these molecules show promise as starting points for the development of new antibiotics, antibacterials, and anti-inflammatory drugs [4]. A first extraction technique was developed to obtain a comprehensive profile of polyphenolic components and enrich the database. The project's novelty lies in applying in silico methods to uncover the physicochemical and ADME properties of these compounds, aiding the design, synthesis, or extraction of new antibacterial and anti-inflammatory drugs, including potential COX-1 inhibitors.

Fondazione INF-ACT

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FP n° 14

AUTOMATIC COMPUTATIONAL PROTOCOL TO EXPLORE G-QUADRUPLEX'S BINDING SITES THROUGH MOLECULAR DYNAMIC SIMULATIONS AND VIRTUAL SCREENING

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G-quadruplexes (G4s) are non-canonical secondary structures of DNA and RNA that play crucial roles in various biological processes1. The G4 core structure is composed by at least two quartets (G-tetrads) of co-planar guanines stacked atop each other's. G4s have recently emerged as promising targets for antibiotic development2 given their role in bacterial growth and replication. However, the discovery of bacterial G4 binders is hindered by the limited data on bacterial G4 structures and the consequent lack of information on their druggable sites.
Here, we present a new automated computational protocol to explore a target macromolecule applied to the structure of the Pseudomonas aeruginosa G4 TET22, for which no prior information on ligand binding nor interaction modes were available. The protocol (i) scans the quadruplex to find all the potential binding pockets using mixed-solvent molecular dynamics (Mixed-MD) simulations and (ii) drives drug design through probes growing up to hits by Virtual Screening. Mixed-MD simulations were set up with molecular probes (MW<150 Da) as co-solvent units. From the analysis of the Linear Interaction Energy (LIE) between the quadruplex and the molecular probes, and the time persistence of these interactions, TET22 potential hotspots were identified. Combining the probes with the lowest LIE and the highest time persistence, different fragments were designed and then used as co-solvent units in a new set of Mixed-MD simulations. Fragments exhibiting the strongest LIE and persistence of interaction were further selected as substructures for filtering a commercial compound library of 5 million molecules. Following filtering and docking based virtual screening, 11 molecules were identified as potential TET22 binders and are currently under biophysical testing.

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FP n° 15

THE GOLD-ALLENE SYSTEM FOR THE FUNCTIONALIZATION OF 7- AND 4-MEMBERED RINGS

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The Au-assisted electrophilic activation of unsaturated hydrocarbons has gained significant recognition over the past two decades for the functionalization of countless chemical platforms.[1] The use of Au-cumulene chemistry for the functionalization of small (4-membered) and medium (7-membered) size rings, among the most challenging to be synthesized and functionalized, will be presented.

Tropone and tropolone compounds are emerging organic platforms for creating chemical diversity/complexity in the area of pharmaceutical ingredients. A site-selective alkylation of α-aminotropones was effectively realized via Au(I)-catalyzed electrophilic activation of allenamides and allenyl ethers, yielding up to 85% in 30 examples. A dedicated and combined spectroscopic and computational investigation accounted for both chemo- and regioselective profiles of the protocol.[2]

Bicyclobutanes are among the most highly strained isolable organic compounds and their associated low activation barriers to reactivity make them intriguing building-blocks in organic chemistry. A highly efficient [2+2] cycloaddition of bicyclobutanes and Au-activated allenamides and allenyl ethers was developed giving rise to a series of diversely decorated [1.1.2]-bicyclopentanes (25 examples, yields up to 93%) amenable for further functionalizations.[3]

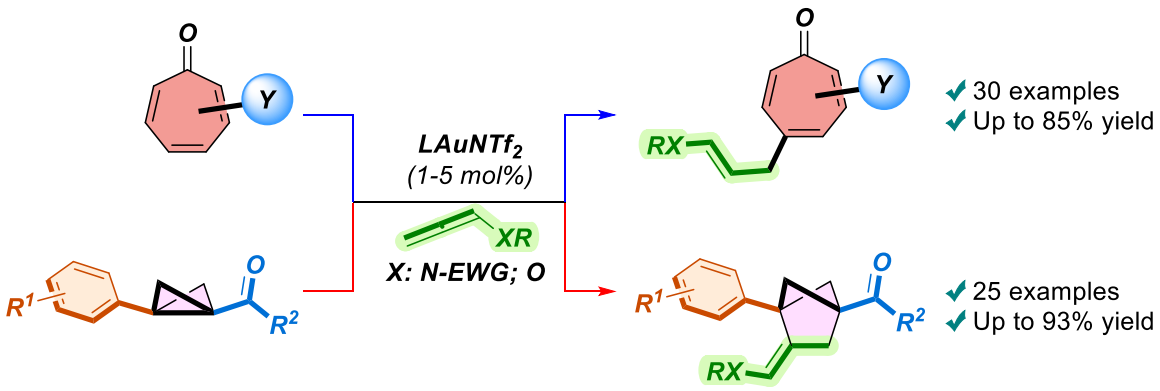

Figure 1. Au-allene system for the functionalization of 7- and 4-membered rings.

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FP n°16

DIRECT ACCESS TO BENZOLACTAMS AND BENZOLACTONES VIA NICKEL CATALYZED CARBONYLATION WITH CO_2

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During last years, CO_2 emerged as a safe and effective C1 source in organic synthesis. In this scenario, despite the undoubtful synthetic value, carbonylation processes still remain confined to a handful number of protocols such as: alkene and amine hydroformylations and amino- or alkoxycarbonylations.[1] In addition, carbonylations with CO_2 commonly require direct reduction to carbon monoxide by means of harsh reaction conditions.[2]
To this aim, a new Ni- catalyzed cross-electrophile coupling (XEC) strategy is exploited in a fruitful way, for the preparation of amides and esters using CO_2 as the carbonyl source. The process has been designed for the synthesis of polysubstituted isobenzofuranones and *N*-aryl isoindolinones in good to high yields (29 examples, Fig. 1).[3] A pivotal role is played by the $AlCl_3$ additive, which already resulted competent in Ni-catalyzed carbonylation protocols for formal CO_2 to CO permutation, as well as for carboxylation strategies in C-C bonds formation reactions.[4,5] Indeed, in this case, investigation on the role of $AlCl_3$ revealed that it accounts both as CO_2 activator in the carboxylation step and as a promoter for the formation of a transient carbamate, acting as a protecting group of the free amine moiety.

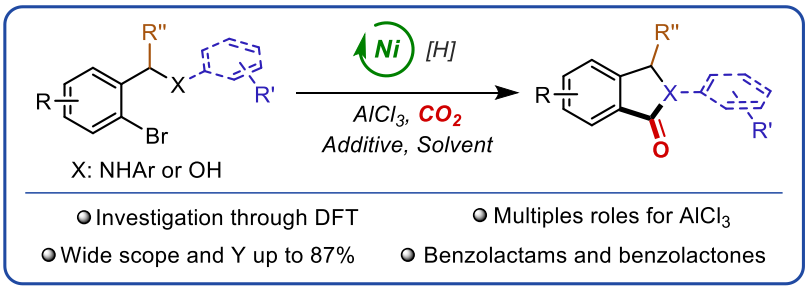

Figure 1. Carbonylative Ni-catalyzed XEC under $AlCl_3$ Lewis acid assistance.

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FP n°17

DEVELOPMENT OF A ONE-POT, SOLVENT-FREE REACTION FOR THE SYNTHESIS OF FLUOROQUINOLONE ANTIBIOTIC CHEMICAL CORE

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Fluoroquinolones are well-known for their broad-spectrum antibacterial properties, effectively targeting both aerobic Gram-positive and Gram-negative pathogens. Their versatility and potent bactericidal effects make them widely used in treating various infections, including urinary tract, gastrointestinal, respiratory, and sexually transmitted diseases.[1] However, the traditional production of these compounds often relies on chemical processes that are neither environmentally friendly nor sustainable. These methods typically involve multistep reactions with a low overall yield, extended reaction times, high reaction temperatures, and the use of volatile organic solvents. To address these limitations, a one-pot, solvent-free synthetic method was being actively explored. This approach simplifies the production process by combining multiple reaction steps into a single one, thereby reducing waste, streamlining workflows, and enhancing the overall efficiency of the synthesis. The solvent-free nature of this method aligns with the principles of green chemistry, minimizing environmental impact and promoting safer chemical practices. Moreover, the use of microwaves[2] allows for a drastic reduction in reaction times and energy consumption of conventional heating. Such advancements represent a promising step toward more sustainable approaches in pharmaceutical manufacturing.

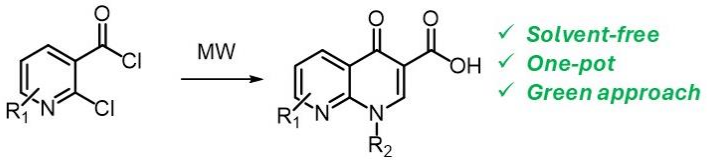

Figure 1. Generic scheme for the innovative approach in the synthesis of fluoroquinolone antibiotic chemical core.

This project is supported by P2022CKMPW and MFAG 2017-ID20160.

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FP n° 18

STUDY OF THE CISS EFFECT TROUGH CHIRAL PEPTIDE DYADS

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Optical control and readout of qubits are of outstanding importance in the emerging field of quantum technology.
In this context we provide the synthesis of a substrate which serves as reliable model for studying the chirality-induced spin selectivity (CISS) effect at the molecular level [1], which is the filtering effect of electron spin when involved in chiral pathways.
The substrate is a chiral dyad composed of quantum dots (QDs) as donor and fullerene as acceptor connected by a saturated peptide bridge. The synthesis involves the formation of peptide bridge made of two aminoacidic building blocks, capable of facilitating electron transfer (ET) when incorporated in a short chain [2], followed by the coupling with fullerene via the Prato reaction. To complete the dyad, the final step is the exchange reaction of this substrate as a ligand on the surface of CdSe nanoparticles.
To further enhance the sensibility of the molecular model, the next step is the formation of a triad with molecular qubit which should provide an unambiguous signal upon detection. We are studying the synthesis of macrocyclic ester ligands to prepare spin-coherent vanadyl complexes [3] that could act as qubits.

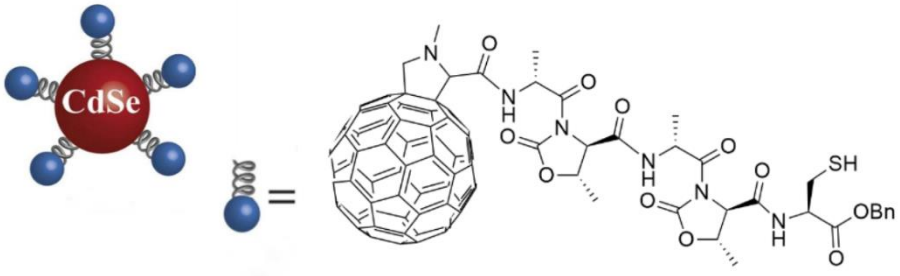

Figure 1.

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FP n° 19

WASTE-MINIMIZED ACCESS TO DIARYLAMINES AND TRIARYLAMINES VIA C*SP*^{2}–N COUPLING UNDER BATCH AND FLOW CONDITIONS

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A waste-minimized strategy for synthesising diarylamines and triarylamines *via* Buchwald-Hartwig coupling is herein reported. These structural motifs rank among the top 20 most prevalent functional groups in biologically active molecules, and they are widely used in fields ranging from medicinal chemistry [1] to materials science [2]. In this work, the heterogeneous catalyst Pd/C was effectively employed under batch conditions and packed into the reactor for the flow setup. Our waste-reduction strategy utilises an azeotropic mixture of cyclopentyl methyl ether (CPME) derived from petrochemical waste and water. To enhance process circularity, the heterogeneous catalyst, phosphine-based ligand, and CPME were recovered and reused. The use of a biphasic CPME azeotrope as the reaction medium facilitated the process under flow conditions by enabling the solubilisation of all reaction components. Final product isolation was achieved thanks to an in-line liquid-liquid separator, which allowed for a significant reduction in waste generation.

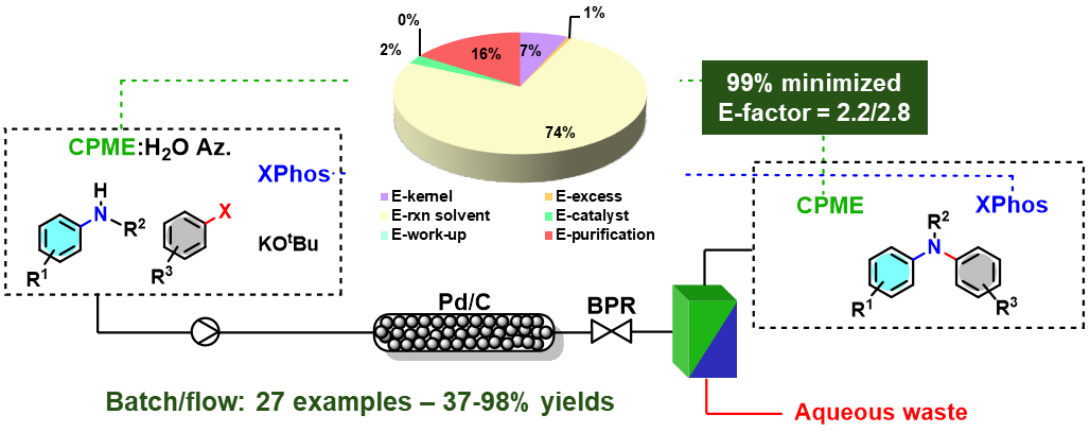

Figure 1. Graphical Abstract.

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