



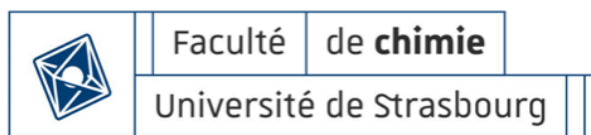
3rd SUSTAINABLE CHEMISTRY DAY

21 NOVEMBER 2025 —

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WHAT'S THE PROGRAM ?

8h15	WELCOME
8h45	OPENING
SESSION 1	<i>Chairs - Laure BENHAMOU & Stefan CHASSAING</i>
9h	Pascal MÉTIVIER
9h40	ORAL COMMUNICATIONS- session I
	9h40 OC1 - Adam DUONG
	9h55 OC2 - Romain PERTSCHI
	10h10 OC3 - Floriane RISCHARD
	10h25 OC4 - Mohamed R IMACHE
10h40	Laurence HECQUET
11h20 - FLASH PRESENTATIONS	CHIMIE VERTE ACADEMY
	FP1 - Pauline FRAMBOURG
	FP2 - Anatole HIDALGO
	FP3 - Emma DEMATHIEU
	FP4 - Hossam FAROUK
	FP5 - Mila MOREAU
11h35	LUNCH & POSTER SESSION
SESSION 2	<i>Chairs - Dominique AGUSTIN & Gregory CHATEL</i>
13h45	ORAL COMMUNICATIONS - session II
	13h45 OC5 - Aghiles Karim AISSAT
	14h OC6 - Alexis PERROT
	14h15 OC7 - Marie-Hélène PIETRARU
	14h30 OC8 - Maxime HOURTOULE
	14h45 OC9 - Samuele MARINARI
	15h OC10 - Elliott JUNG
	15h15 OC11 - Lénaïck HERVÉ
15h30	COFFEE BREAK
SESSION 3	<i>Chair - Franck LAUNAY</i>
16h	Mathieu LEPAGE
	<i>Young Researcher laureate of the DivCD award 2024</i>
16h25	Thomas DARDÉ
	<i>Young Researcher laureate of the DivCD award 2025</i>
16h50	Sylvain GUIZZETTI
17h30	PRIZES & CLOSING REMARKS

3rd SUSTAINABLE CHEMISTRY DAY – 21 NOVEMBER 2025, STRASBOURG

TALKS

DECARBONATION OF THE CHEMICAL INDUSTRY – FACTS, CHALLENGES, AND RESEARCH OPPORTUNITIES

Dr Pascal MÉTIVIER

Consultant, professor, previous research director at Syensqo, Solvay and Rhodia

The chemical industry can be considered as the « mother » of other industries since most products we use on a daily basis have gone through a chemical step during their manufacture. As a consequence emissions of green house gas linked to the chemical industry, direct and indirect, are not negligible and contribute to climate change. We will review some facts relative to emissions linked to the chemical industry, review the challenges that the industry is facing if we want to massively decarbonize the industry and also what are the key fields where research and innovation is needed to bring new solutions to support this decarbonation.



BIO – Pascal MÉTIVIER is a scientific consultant and professor with a distinguished career as research director at Syensqo, Solvay, Rhodia, and Rhône-Poulenc. Over 40 years, he led global research and innovation in Europe, UK and Asia (China). He now shares his expertise through teaching sustainability via the French School of Chemistry (Fédération Gay-Lussac) and advises pioneering companies in science and advanced technology.

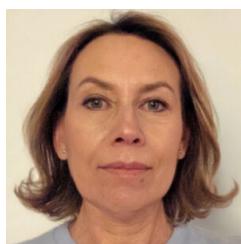
Biocatalysis : advances and applications in chemical synthesis

Laurence Hecquet

*Institut de Chimie de Clermont-Ferrand (ICCF- UMR6296), Université Clermont Auvergne
63177 Aubière Cedex, France
laurence.hecquet@uca.fr*

Biocatalysis has become an important tool in chemical synthesis even in pharmaceutical, agricultural, food and chemical industries, allowing access to small and complex molecules with high levels of activity and selectivity and with low environmental impact.¹ Many limitations have now been resolved through integrative, multidisciplinary approaches based on key discoveries in protein engineering combining computational design and molecular biology techniques affording increasingly powerful enzymes.² In addition, the design and development of artificial biocatalytic cascades in one-pot avoid intermediate purification and allow equilibrium shift and cofactor regeneration.

The enzymatic pathways developed in my group relies on such integrative approaches particularly for the synthesis of unsymmetrical α -hydroxyketones found in diverse pharmaceuticals and agrochemicals. While the chemical synthesis of these compounds requires uneconomical steps for protective group manipulations, carboligases such as thiamine dependent enzymes are particularly suitable and efficient to obtain α -hydroxyketones. We showed that the thermostable Transketolase (TK) from *Geobacillus stearothermophilus*³ has great advantages for obtaining these compounds. The broadening of its substrate spectrum by rational mutagenesis and the coupling of the best efficient variants with auxiliary enzymes in one pot allow to obtain at preparative scale many valuable α -hydroxyketones.⁵⁻⁸



BIO – Laurence HECQUET is a Professor of Bioorganic Chemistry at the University of Clermont Auvergne and co-Director of the Institute of Chemistry of Clermont-Ferrand. Her research lies at the interface of biology and chemistry, focusing on enzyme-based synthesis of chiral compounds using carboligases, with work on mutagenesis, enzymatic screening, and cascade reactions. Author of around 100 publications, she leads multiple research projects at regional, national, and European levels and maintains strong industrial collaborations. A distinguished member of the French Chemical Society since 2015 and a member of the National Committee of Universities, she also chairs the CBSO network and contributes actively to European initiatives, including chairing the 2023 BIOTRANS symposium.

¹ A. O'Connell et al, *Chem. Soc. Rev.*, **2024**, 53, 2828-2850.

² E.J. Hossack et al, *ACS Catal.*, **2023**, 13, 12436-12444.

³ J.Abdoul Zabar et al, *Adv. Synth. Catal.*, **2013**, 355, 116-128.

⁴ T. Saravanan et al., *Angew. Chem. Int. Ed.*, **2017**, 56, 5358–5362.

⁵ M. Lorillière et al, *ACS Catal.*, **2019**, 9, 4754-4763. IF 12.35

⁶ N. Ocal et al, *Org. Process Res. Dev.*, **2020**, 24, 769–775.

⁷ G. Arbia et al, *Green Chem.*, **2024**, 26, 7320-7330.

⁸ C. Gadona et al, *ACS Catal.*, **2025**, 15, 10, 7979–7992

FLOW CHEMISTRY AS A TOOL FOR DRUG DISCOVERY & EARLY PROCESS DEVELOPMENT

Sylvain Guizzetti

*Bioparc, 850 bld Sébastien Brant, BP 30170, 67405 Illkirch Cedex, France
sguizzetti@novalix.com*

Flow chemistry is increasingly recognized as a transformative platform for the synthesis and development of pharmaceutical agents, and several recent industrial implementations—supported and endorsed by regulatory bodies such as the FDA—underscore its growing relevance. Beyond improved heat and mass transfer, enhanced control of reaction parameters, and inherent safety advantages, continuous flow processing offers more sustainable and resource-efficient manufacturing routes. These features align closely with the pharmaceutical sector's shift toward greener and more agile development strategies.

A brief comparison between batch and flow processing will highlight how continuous methods can reduce waste, improve energy efficiency, and simplify scale-up, reinforcing their value in early process development.

This framework sets the stage for practical examples drawn from drug discovery programs. Continuous flow systems have proven especially powerful for transformations that are difficult to manage in batch. Organometallic reactions benefit from precise control over highly reactive intermediates and safer handling of sensitive reagents, while photochemical processes gain from uniform irradiation and well-defined residence times. These advantages enable rapid route exploration, streamlined reaction optimization, and smooth transfer from milligram to multigram scale.

The PIPAc project, carried out by a consortium including Novalix, Alysophil, Bruker, and De Dietrich Process Systems, will finally exemplify how continuous synthesis can be coupled with advanced automation for API manufacturing. By integrating real-time analytical monitoring, data-driven control strategies, and modular reactor–separator architectures, the platform aims to develop intelligent and adaptive continuous workflows. Demonstrated applications include the continuous production of clinically relevant APIs such as propofol and fentanyl, illustrating how the convergence of flow chemistry and artificial intelligence can enable more flexible, efficient, and sustainable pathways to essential medicines.



BIO – Sylvain GUIZZETTI is a senior chemist with over 20 years of experience in organic synthesis, early process development, and flow chemistry. He holds an engineering degree from ENSCMu and a PhD in organic chemistry from the University of Strasbourg, conducted in collaboration with Bayer CropScience and the CNRS under the supervision of Charles Mioskovski and Alain Wagner. He began his career as a project manager in medicinal chemistry at NovAliX, before specialising in process development and driving the implementation of flow technologies within the company. He now leads the Flow & Process Chemistry department at NovAliX, overseeing multi-site operations, innovation strategy, and collaborative research. His work focuses on bridging early discovery and scalable solutions to accelerate pharmaceutical development.

ELECTRON-POOR BUTENOLIDES: A BIO-BASED ALTERNATIVE TO ACRYLATES AND A MISSING LINK IN THEIR FAMILY TREE

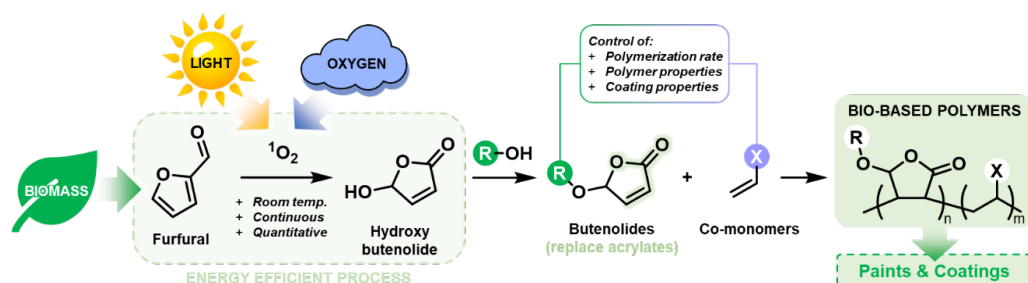
M. L. Lepage,^{* 1,2} G. Alachouzos,² J. G. H. Hermens,²
N. Elders,³ K. J. Van Den Berg³ and B. L. Feringa^{* 2}

¹ Current address: LHFA, CNRS, Université de Toulouse, France

² Stratingh Institute for Chemistry, ARC CBBC, University of Groningen, The Netherlands

³ Dept. Resin Technology, AkzoNobel Car Refinishes BV, Sassenheim, The Netherlands
mathieu.lepage@cnrs.fr

Photo-oxidation of waste biomass-derived furfural with singlet oxygen affords hydroxy butenolide, a singly reduced derivative of maleic anhydride, with minimal waste in matter and energy. This efficient process can be performed both in batch and flow setups.¹ Hydroxy butenolide can be further derivatized through its acetal moiety, for instance by condensation or esterification with a variety of (potentially bio-based) alcohols and acids, respectively. The resulting butenolides are cyclic acetals which incorporate an acrylate motif and thus constitute a sustainable alternative to acrylate-based polymers used in the coatings industry. We have used these butenolides to design a fully bio-based coating system in which all the components are derived from renewable sources.²



The variability in the substituents and in the co-monomers offers a control on both the reactivity during radical polymerization and on the properties of the coatings obtained after cross-linking. We rationalized the reactivity of butenolides using a combination of kinetics experiments and DFT computation.³ The versatility of this new platform holds many promises for bio-based polymers and coatings, and beyond that for functional materials.

¹ Hermens *et al.*, Development of a modular photoreactor for the upscaling of continuous flow photochemistry. *React. Chem. Eng.* **2022**, 7 (11), 2280. DOI: [10.1039/d2re00310d](https://doi.org/10.1039/d2re00310d)

² Hermens *et al.*, A sustainable polymer and coating system based on renewable raw materials. *Green Chem.* **2022**, 24 (24), 9772. DOI: [10.1039/d2gc03657f](https://doi.org/10.1039/d2gc03657f)

³ Lepage *et al.*, Electron-Poor Butenolides: The Missing Link between Acrylates and Maleic Anhydride in Radical Polymerization. *J. Am. Chem. Soc.* **2023**, 145 (31), 17211. DOI: [10.1021/jacs.3c04314](https://doi.org/10.1021/jacs.3c04314)

ORGANIC CATALYSIS FOR POLYMERIZATION OF ALKYL MUCONATES AS A BIO-BASED ALTERNATIVE OF ACRYLATES

THOMAS DARDÉ¹, XAVIER SCHULTZE², DANIEL TATON¹

¹ Laboratoire de Chimie des Polymères Organiques (LCPO), Université de Bordeaux, CNRS, Bordeaux INP, UMR 5629, 16 av. Pey Berland, 33607 Pessac cedex.

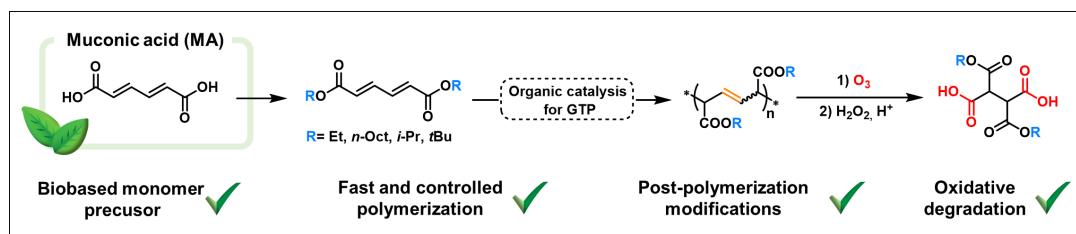
² L'Oréal Research & Innovation, 1 Avenue Eugène Schueller, 93601 Aulnay Sous-Bois.
Email : thomas.darde@u-bordeaux.fr

The development of an "ideal plastic", *i.e.* a polymer that is bio-based, degradable or recyclable after use, and also offers versatile options for chemical post-modification, remains a significant challenge in modern polymer science.¹

Our project focuses on designing a synthetic methodology that enables the rapid polymerization of bio-based monomers, yielding structurally well-defined polymers in less than one minute at room temperature via organic group transfer polymerization (O-GTP). The ultimate goal is to create a polymer platform with programmable and rapid chemical degradation to reduce dependence on fossil resources and minimize environmental impact.

To address this challenge, we explore the potential of dialkyl muconate esters, monomers derived from bio-based muconic acid (2,4-hexadienedioic acid), which uniquely combine conjugated diene and dicarboxylic acid functionalities.^{2,3} These monomers offer multiple advantages, including precise control over polymer structure, tunable alkyl side groups, modular post-polymerization chemical modifications, facile degradation, and sustainable bio-based sourcing.

We demonstrate that polymuconates represent a versatile platform of bio-based polymers, characterized by ease of chemical modification and degradability under user-friendly experimental conditions.⁴ This study highlights the flexibility of O-GTP as a versatile method to create functional materials that can meet industrial performance needs, while addressing environmental challenges.



¹ Coates, G. W.; Getzler, Y. D. Y. L. *Nat Rev Mater* **2020**, 5 (7), 501–516.

² Khalil, I.; Quintens, G.; Junkers, T.; Dusselier, M. *Green Chem.* **2020**, 22 (5), 1517–1541.

³ Ver Elst, C.; Maes, B. U. W. In *Reference Module in Chemistry, Molecular Sciences and Chemical Engineering*; Elsevier, **2024**; B9780443157424000000.

⁴ Dardé, T.; Diomar, É.; Schultze, X.; Taton, D. *Angew Chem Int Ed* **2024**, 63 (50), e202411249.

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ORAL COMM

Melamine Valorization into Sustainable Cyamelurate-Based Materials: Toward CO₂ Capture and Sensing

Adam Duong

Junior Professor Chair

University of Picardie Jules Verne, 10 rue Baudelocque, 80000 Amiens, France

adam.duong @u-picardie.fr,

Transforming waste into functional materials is a promising pathway for sustainable chemistry. In this work, melamine is valorized into cyamelurate via a simple, solvent-free process for the synthesis of Metal–Organic Frameworks (MOFs).^{1,2} Coordination with lanthanides yields porous materials effective for CO₂ capture, contributing to carbon neutrality. Coordination with transition metals leads to two-dimensional materials with reversible chromic properties, enabling potential sensing applications.³ This project highlights an integrated green chemistry approach: waste valorization, resource-efficient processes, and the design of advanced materials for energy and environmental challenges.

Keywords : Sustainable chemistry; Waste valorization; Cyamelurate; MOFs; CO₂ capture; Functional materials.

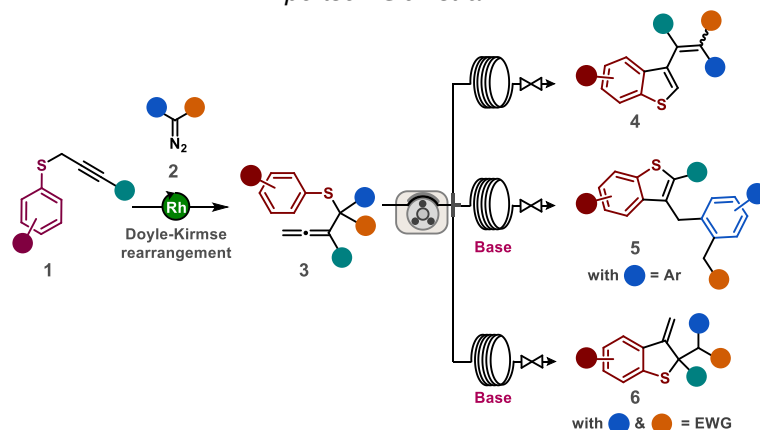
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2. Mohan, Midhun; Essalhi, Mohamed; Durette, David; Rana, Love Karan; Ayevide, Follivi Kloutse; Maris, Thierry; Duong, Adam. *ACS Appl. Mater. Interfaces*. **2020**, *12*(45), 50619-5062.
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DIVERGENT SYNTHESIS OF BENZOTHIOPHENE DERIVATIVES IN CONTINUOUS FLOW

Timoth  Maujean, Camille Van Wesemael, Patrick Wagner, Mihaela Gulea,
Romain Pertschi*

Facult  de pharmacie, Universit  de Strasbourg, 74 route du Rhin, 67400, Illkirch,
rpertschi@unistra.fr



One of the major challenges in drug discovery is to synthesize innovative bioactive compounds that explore novel chemical spaces. However, obtaining a large diversity of molecules using classical organic chemistry methods is time-consuming and expensive. Indeed, these methods typically entail long, linear, multistep syntheses that offer only a few points of structural divergence. Consequently, chemical libraries are restricted in terms of structural diversity. Thus, Diversity Oriented Strategies as well as cascade reactions have always been highly sought after since they provide a rapid access to a large variety of complex molecules by assembling simple and readily available starting materials.¹ These strategies not only allow efficient access to unique molecular architectures, but, thanks to their step and atom economy, they are also aligned with more sustainable approaches to drug production, making them a powerful “Swiss army knife” for the discovery and synthesis of pharmaceutical compounds. In this context, the Doyle–Kirmse rearrangement represents a good example of such a strategy, as it can lead to a large diversity of highly functionalized sulfides **3**, starting from readily available thioethers **1** and diazo compounds **2**.² Despite the high potential of this reaction to generate diversity, only a few post-Doyle–Kirmse transformations have been developed.³ In this context, a modular and divergent approach based on post-Doyle–Kirmse cascade reactions has been developed using continuous flow chemistry. Depending on the reaction conditions and the nature of the starting materials, these cascades selectively yield various benzothiophene derivatives (**4**, **5**, **6**) that are of interest in drug discovery.⁴

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2. a) Peng, L.; Zhang, X.; Wang, J. *Angew. Chem. Int. Ed.* **2007**, *46*, 1905–1908; b) West, T. H.; Spoehrle, S. S. M.; Kasten, K.; Taylor, J. E.; Smith, A. D. *ACS Catal.* **2015**, *5*, 7446–7479.

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GREEN SYNTHESIS OF FERULIC ACID ESTERS FOR NEXT-GENERATION COSMETIC FORMULATIONS

Floriane Rischard^{1,2}, Ecaterina Gore¹, Amandine Flourat², Géraldine Savary¹

1. URCOM, Université Le Havre Normandie, 25 rue Philippe Lebon, 76600 Le Havre

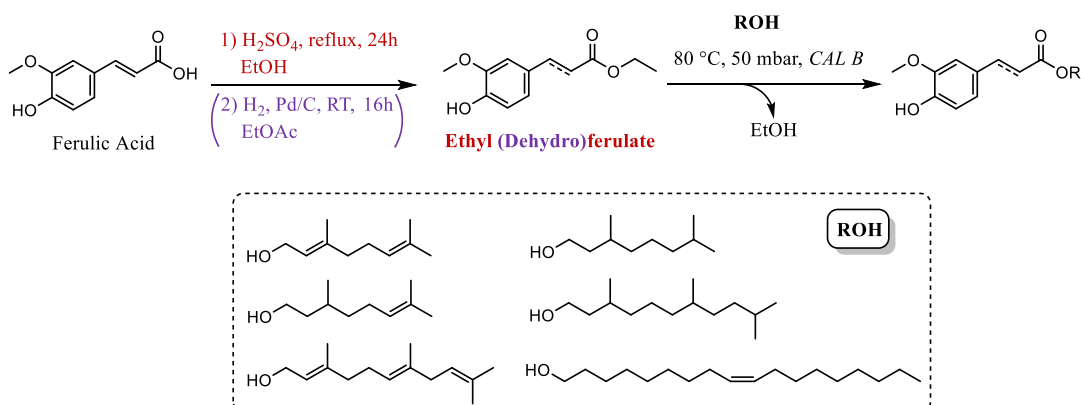
2. URD ABI, AgroParisTech, 3 rue des Rouges-Terres, 51110 Pomacle

floriane.rischard@univ-lehavre.fr

Cosmetic products often rely on a multitude of ingredients to achieve their desired functions. Many of these are petroleum-based, raising concerns about their environmental footprint, possible health risks, and the increasingly complex formulations that can unsettle consumers.^{1–4} To overcome these challenges, a new class of multifunctional biobased cosmetic ingredients was introduced.⁵

Our work focused on the valorization of renewable ferulic acid, which can be found in non-neglectable quantities in many agricultural by-products. By esterifying ferulic acid with diverse bio-based fatty chains, we synthesized a library of twelve derivatives that combine new emollient properties with the intrinsic protective activities of ferulic acid, including antioxidant, anti-UV and antimicrobial effects.

All syntheses were performed following green chemistry principles, and the resulting compounds were systematically assessed. The derivatives displayed protective and sensory properties competitive to conventional commercial ingredients, thereby opening pathways toward more sustainable and multifunctional cosmetic formulations.



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(2) Ma, X. *et al. Journal of Cosmetic Dermatology* **2021**, 20 (1), 195–203.

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(4) Ouchene, L. *et al. J Cutan Med Surg* **2019**, 23 (6), 648–649.

(5) Rischard, F. *et al. ACS Sustainable Chem. Eng.* **2023**, 11 (48), 16955–16964.

SYNTHIA™: Revolutionizing Sustainable Organic Chemistry through Computational Intelligence

Mohamed R. IMACHE & Aurélie CHAMBON

mohamed-rabah.imache@merckgroup.com

aurelie.chambon@merckgroup.com

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Chemical Valorization of Viticultural Waste: Stilbene Extraction and Photoprotection Strategies

Aghiles Karim AISSAT^a, Audrey DAMIENS^a, Elea COLLANGE^{ab}, Sylvain SCHNEE^c, Marion ZWINGELSTEIN^c, Micheline DRAYE^a, Katia GINDRO^c, Grégory CHATEL^{a,*}

^a Univ. Savoie Mont Blanc, CNRS, EDYTEM, 73000, Chambéry, France

^b PEPS SAS, Bourget-du-Lac, France

^c Mycology Group, Agroscope of Changins, 1260 Nyon, Switzerland

aghiles-karim.aissat@univ-smb.fr

In 2022, global grape production reached approximately 110 million tons, generating significant amounts of viticultural waste¹. Poor management of these residues raises major environmental concerns. Within this context, the VITIVALO project aims to develop sustainable strategies for managing vine by-products through chemical valorization.

Vine shoots, produced annually in large quantities during pruning, represent a promising yet underexploited biomass. Their valorization is limited by the photosensitivity of key bioactive stilbenes, mainly trans-resveratrol and trans-viniferin. To address this issue, ethanol/water reflux extractions were performed to maximize compounds recovery and the presence of stilbenes was confirmed by UPLC-DAD analyses. Extract stability was then assessed under accelerated aging conditions (up to 120 minutes) using a Suntest device. Upon UV exposure, rapid isomerization of trans-stilbenes into their less active cis forms occurred within 15 minutes. To mitigate this phenomenon, three mixtures incorporating various biomasses at different ratios were developed and tested. These mixtures reduced isomerization by approximately 50%. Moreover, antifungal assays against *Botrytis cinerea* revealed minimum inhibitory concentrations ranging from 1 to 10 mg/mL, depending on the extract.

Overall, the chemical valorization of vine shoots represents a key step toward more sustainable viticulture. The incorporation of protective biomasses appears to be a promising strategy to enhance the stilbene photostability, extending their potential applications in agricultural and biobased systems.

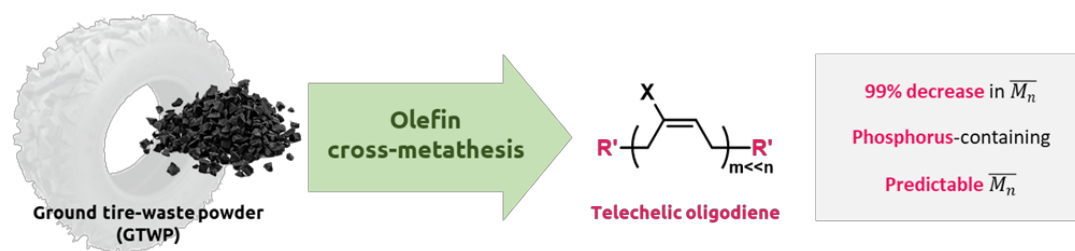
(1) OIV, S. State of the World Vine and Wine Sector 2021. *Int. Organ. Vine Wine Dijon Fr.* **2022.**

PREDICTABLE TELECHELIC OLIGODIENES FROM TIRE WASTE BY OLEFIN METATHESIS DEPOLYMERIZATION

Alexis Perrot,* Julien Renault, Charles Jambou, Isabelle Dez*

Institut CARMEN UMR 6064, Université Caen Normandie, ENSICAEN, CNRS, INSA Rouen Normandie, Univ Rouen Normandie, 6 bd Maréchal Juin, 14000 Caen, France
alexis.perrot@ensicaen.fr

Each year, hundreds of millions of tons of plastic waste are generated globally, including approximately one billion end-of-life tires.^{1,2} To mitigate the environmental impact of this waste, the chemical valorization of polydienes found in tires offers a promising route to obtain reusable raw materials. In particular, olefin cross-metathesis using ruthenium-based catalysts represents a powerful method to simultaneously depolymerize and end-functionalize the polymers, yielding functional oligomers amenable to further processing.^{3,4} Here, we report our efforts to synthesize phosphorus-containing oligomers from rubber waste through olefin cross-metathesis. Specifically, we demonstrate the efficient depolymerization of high-molar-mass linear polyisoprene into phosphonate-terminated oligoisoprene ($\overline{M}_n = 5.4 \text{ kg mol}^{-1}$). Remarkably, the reaction also proceeds on vulcanized rubber networks, affording oligomers with $\overline{M}_n = 10 \text{ kg mol}^{-1}$ despite the presence of additives and crosslinks. We developed a simple mathematical model correlating the molecular weight of the products with the extent of reaction, enabling fine control over the degree of polymerization.⁵ This framework paves the way towards the design of well-defined materials from phosphorus-containing oligomers derived from tire waste.



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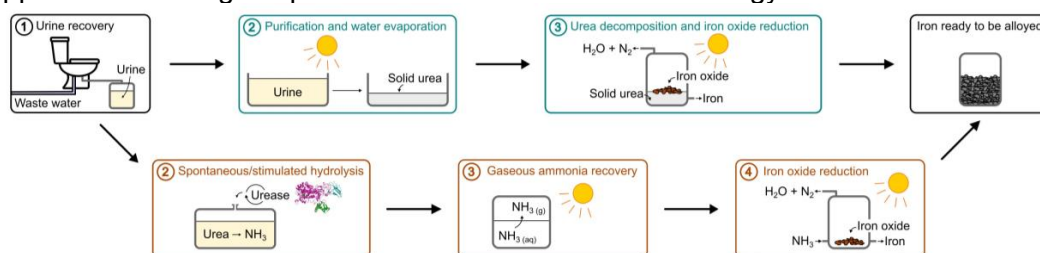
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LOW-TECH PROCESSES FOR SOLAR METALLURGY

Marie-Hélène Pietraru, Marion Luu, Sébastien Lachaize, Julian Carrey

Laboratoire de Physique et Chimie des Nano-Objets (LPCNO), Université de Toulouse,
INSA, CNRS UMR 5215, UPS, 135 av. de Rangueil, 31077 Toulouse Cedex 4
pietraru@insa-toulouse.fr

Green growth is the prevailing paradigm to provide solutions to the climate crisis: technological innovation should allow decoupling between GDP growth and detrimental environmental consequences. Degrowth scholars have however questioned the feasibility of this decoupling¹, and advocate instead for the discontinuing of the pursuit at all cost of GDP growth, toward steady-state economies. While degrowth has gained traction in economics, the question remains quite open regarding natural sciences²: what sociotechnical system would be appropriate in a context of degrowth? The *low-tech* framework is adequate for fueling reflection on this question, as it encompasses both engineering and sociopolitical facets³, and was here applied to the design of processes for iron and steel metallurgy.



The production of steel starts by the reduction of iron oxide into metallic iron, a reaction which relies nowadays mostly on fossil resources and is highly carbon emissive. We envisioned instead the use of solar concentration as a source of heat, and urine as a source of a reducing agent, ammonia⁴, both process inputs that are accessible, equitably distributed, renewable, and bio-sourced. Two pathways were explored, starting from solid or aqueous urea. First, direct pyrolysis fueled by the residual heat provided by light concentration allowed thermal decomposition of solid urea to NH₃. Second, the urease-catalyzed hydrolysis of urea in urine was modelled by an aqueous solution of urea (20 g/L). The generated ammonia was transferred to the reduction reactor as a gas thanks to a thermal process, without any further separation from air or water vapour. The two pathways afforded excellent iron oxide to iron conversions, respectively as high as 90% after 18 min under light flux and 98% after 8 min.

¹ Vogel, J.; Hickel, J. Is Green Growth Happening? An Empirical Analysis of Achieved versus Paris-Compliant CO₂-GDP Decoupling in High-Income Countries. *The Lancet Planetary Health* **2023**, 7 (9), e759–e769. DOI: [10.1016/S2542-5196\(23\)00174-2](https://doi.org/10.1016/S2542-5196(23)00174-2).

² Hickel, J.; Kallis, G.; Jackson, T.; O'Neill, D. W.; Schor, J. B.; Steinberger, J. K.; Victor, P. A.; Ürges-Vorsatz, D. Degrowth Can Work — Here's How Science Can Help. *Nature* **2022**, 612 (7940), 400–403. DOI: [10.1038/d41586-022-04412-x](https://doi.org/10.1038/d41586-022-04412-x).

³ Carrey, J.; Lachaize, S. La recherche scientifique en Low-Tech : définition, réflexions sur les pistes possibles, et illustration avec un projet de métallurgie solaire. *La Pensée écologique* **2020**, 5(1), 7-7. DOI: [10.3917/lpe.005.0007](https://doi.org/10.3917/lpe.005.0007).

⁴ Luu, M.; Sanglard, B.; Lachaize, S.; Carrey, J. Towards Solar Metallurgy: Iron Ore Reduction by Ammonia under Concentrated Light Flux. *Solar Energy* **2025**, 287, 113250. DOI: [10.1016/j.solener.2025.113250](https://doi.org/10.1016/j.solener.2025.113250).

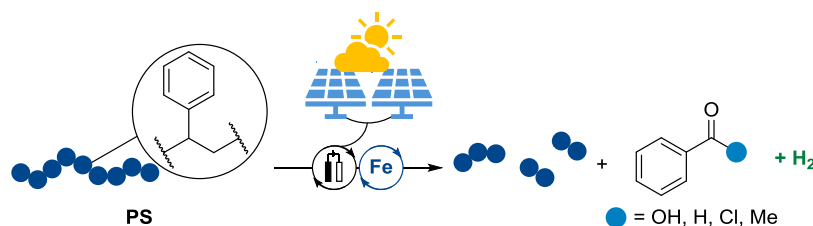
Anodic Commodity Polymer Recycling: The Merger of Iron-Electrocatalysis with Scalable Hydrogen Evolution Reaction

M. Hourtoule, S. Trienes, and L. Ackermann*

*Prof. Dr. Lutz Ackermann, Wöhler Research Institute for Sustainable Chemistry, Georg-August-Universität, Tammannstraße 2, 37073 Göttingen, Germany
Lutz.Ackermann@chemie.uni-goettingen.de*

Plastics are omnipresent in our modern societies, and accumulation of post-consumer plastic waste in our environment represents a major societal challenge and jeopardize wildlife and human health. Hence, methods for plastic waste recycling are in high demand for a future circular economy. Specifically, the degradation of post-consumer polymers, especially for ubiquitous polystyrene, towards value-added small molecules constitutes a sustainable strategy for a carbon circular economy.¹ Despite recent advances, chemical polymer degradation continues to be largely limited to chemical redox agents or low energy efficiency in photochemical processes. To overcome those drawbacks, electrochemistry appears to be an outstanding technology due to its cost-efficiency and scalable nature.²

We herein present a powerful iron-catalyzed degradation of high molecular weight polystyrenes through electrochemistry to efficiently deliver monomeric benzoyl products. The robustness of the ferra-electrocatalysis was mirrored by the degradation of various real-life post-consumer plastics, also on gram scale. The cathodic half reaction was largely represented by the hydrogen evolution reaction (HER). Additionally, the electro-polymer degradation could be fueled by solar energy through a commercially available solar panel, indicating an outstanding potential for a decentralized green hydrogen economy.³



¹ Clark, R. A.; Shaver, M. P. *Chem. Rev.* **2024**, 124, 2617–2650.

² Hourtoule, M.; Trienes, S.; Ackermann, L. *Macromol. Rapid Commun.* **2025**, 2500143.

³ Hourtoule, M.; Trienes, S.; Ackermann, L. *Angew Chem Int Ed* **2024**, 63, e202412689.

Discovery of mild oxidation of heteroaromatic amines applying uncommon and counterintuitive reaction conditions

Samuele Marinari, Claire Fave, Irene Erdelmeier

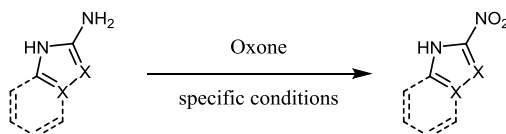
Innoverda, Roissy Charles de Gaulle Cedex, 6 Rue du Noyer, 95734 Roissy-en-France ;
Institut Parisien de Chimie Moléculaire (IPCM), CNRS UMR 8232, Sorbonne Université,
75005 Paris

samuele.marinari@innoverda.com

The selective oxidation of heteroaromatic amines into nitro derivatives has received relatively little attention, despite the broad importance of nitroheteroarenes in pharmaceuticals and related applications.¹ The reported synthetic routes for these compounds generally require drastic reaction conditions and the use of transition-metals.² In particular, the available oxidation methods often rely on highly controlled procedures³ and oxidants that are not widely accessible⁴, limiting their practicality and sustainability.

In this communication, we present a new oxidative protocol in aqueous solution that converts heteroaromatic amines into nitro derivatives under mild, metal-free and environmentally friendly conditions (scheme 1). The transformation employs Oxone® under specifically adjusted aqueous conditions that depart from its conventional use and result in a distinct reactivity profile. This new procedure allows for high selectivity towards the nitro derivative, but can be tuned towards new reaction pathways. Mechanistic implications will be discussed in detail.

This simple and sustainable setup operates efficiently at ambient temperature in aqueous solution, and takes advantage of the low cost, stability and wide availability of Oxone®. This methodology offers a practical and greener alternative to harsher or less accessible oxidation methods for the preparation of valuable nitroheteroarenes.



Scheme 1: Oxidation of heteroaromatic amines to nitro derivatives

¹ Abreu, S. T.; Gelves, L. G. V.; Barreiro, E. J.; Lima, L. M. *J. Braz. Chem. Soc.* **2024**, 35

² Carvalho, D. B.; Costa, P. A. N.; Portapilla, G. B.; das Neves, A. R.; Shiguemoto, C. Y. K.; Pelizaro, B. I.; Silva, F.; Miranda, E. M.; Arruda, C. C. P.; Gaspari, P. D. M.; Cardoso, I. A.; Luccas, P. H.; Nonato, M. C.; Lopes, N. P.; Albuquerque, S.; Baroni, A. C. M. *Eur. J. Med. Chem.* **2023**, 260, 115451

³ Klapoete T. M., Preimesser A., Stierstorfer J., *Propellants Explos. Pyrotech.* **2010**, 35, 1–7.

⁴ Churakov, A. M.; Semenov, S. E.; Ioffe, S. L.; Strelenko, Y. A.; Tartakovskii, V. A. *Mendeleev Commun.* **1995**, 5, 102.

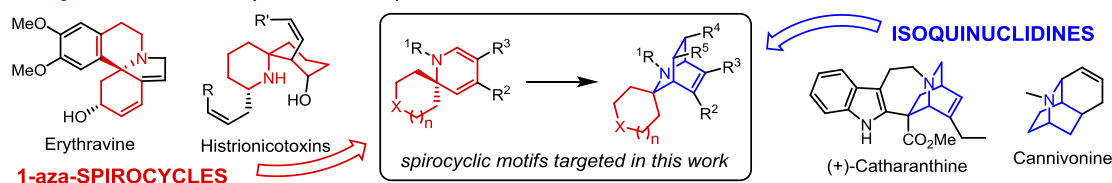
Green synthesis of complex bioinspired spirocyclic motifs

Elliott JUNG,^{1,2} Valérie BÉNÉTEAU,¹ Patrick PALE,¹ Stefan CHASSAING,^{1*} and Christophe GOURLAOUEN^{2*}

¹COSyS, Institut de Chimie de Strasbourg, UMR7177, 67000 Strasbourg, France

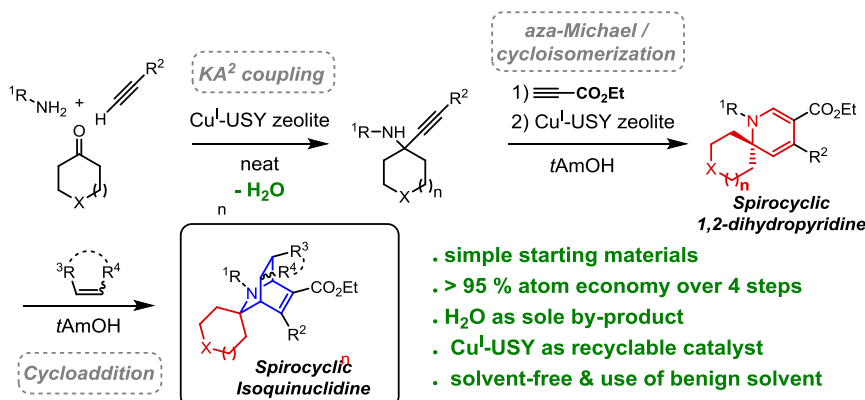
²MSM, Institut de Chimie de Strasbourg, UMR7140, 67000 Strasbourg, France
elliott.jung@etu.unistra.fr

Turning organic synthesis green and sustainable is a pivotal but demanding challenge. Developing synthetic sequences with high atom-/step-efficiencies is a clear alternative, due to the resulting reduction of wastes, energy and number of operations. With these principles in mind, we targeted the synthesis of bioinspired and biologically relevant molecules merging **1-aza-spirocycles** and **isoquinuclidines** (Scheme 1).^{1,2}



Scheme 1

Thus, we wish herein to report our simple and efficient synthetic approach towards such complex **aza-spiro/isoquinuclidine**-based skeletons from **simple starting materials** (Scheme 2). Our approach starts with a 3-steps sequence that furnishes **1-aza-spirocyclic** systems featuring a 1,2-dihydropyridine motif.^{3a} Noteworthy is that 2 of these 3 steps are promoted by a recyclable heterogeneous catalyst, the Cu^I-USY zeolite.^{3b} Finally, the potential of the so-obtained **1-aza-spirocyclic** motif is exploited as a diene to construct the additional **isoquinuclidinic** ring system *via* a formal cycloaddition process.⁴ The elaborated sequence gives access to a high level of complexity with high **atom- and step-economies**, with **water as sole by-product** and using a **recyclable catalyst** as well as suitable solvent conditions (**neat, t-amyl alcohol**), thus meeting most criteria of Green Chemistry.



¹ Lovering, F.; Bikker, J.; Humblet, C. *Journal of Medicinal Chemistry* **2009**, 52(21), 6752-6756.

² Lavaud, C. Massiot, G. *Progress in the Chemistry of Organic Natural Products*; Kinghorn, A.; Falk, H.; Gibbons, S.; Kobayashi, J.; Springer, **2017**, 105, 89-136.

³ a) Schlampen, F.; Plaçais, C.; Starck, E.; Bénéteau, V.; Pale, P.; Chassaing, S. *Journal of Organic Chemistry* **2021**, 86(23), 16593-16613. b) Di, X.; Garnier, T.; Clerc, A.; Jung, E.; Lherbet, C.; Bénéteau, V.; Pale, P.; Chassaing, S. *Molecules* **2024**, 29(23), 5552-5572.

⁴ Wayama, T.; Arai, Y.; Oguri, H. *Journal of Organic Chemistry* **2022**, 87(9), 5938-5951; Martin, R. M.; Bergman, R. G.; Ellman, J. A. *Organic Letters* **2013**, 15(3), 444-447.

Unraveling the Mechanism of HMF Oxidation through a Colloidal Nanocatalyst Approach

Lénaïck Hervé^{1†}, Franck Rataboul¹, Catherine Pinel¹, Amandine Cabioc², Maria Fernandez Espada Pastor², Laurent Djakovitch^{1*}

¹IRCELYON, CNRS, 69626 Villeurbanne, France

²IFP Energies nouvelles, 69320 Solaize, France

* laurent.djakovitch@ircelyon.univ-lyon1.fr

† lennaick.herve@ircelyon.univ-lyon1.fr

The work presented here is performed in the context of the PEPR BBEST-FURFUN program, focused on the valorization of bio-sourced furanic derivatives. Our studies aim at developing efficient and sustainable catalytic oxidation of 5-hydroxymethylfurfural (HMF) for producing high-value compounds such as 2,5-furandicarboxylic acid (FDCA) and 2,5-diformylfuran (DFF). Most reported oxidation methods predominantly use efficient heterogeneous noble metal catalysts with soluble bases, but a deep understanding of the catalytic system is still needed to optimize the processes.¹ Quasi-homogeneous catalysis, based on stable metallic colloids as nanocatalysts, provides a well-defined environment to identify active sites to study reaction mechanisms, and has been applied for the first time to HMF oxidation under mild conditions.²

Nanocatalysts in the form of PVP-stabilized Pd nanoparticles (1.86 ± 0.07 nm) were synthesized in water.³ Catalytic oxidation of HMF was carried out under air flow in water (0.5 wt% HMF) with Na_2CO_3 (1.2 eq./HMF) at 80 °C. Complete HMF conversion was achieved within 48 h, with FDCA selectivity exceeding 80%. The colloidal system allows direct access to the intrinsic behavior of the active metal, free from support effects, enabling detailed mechanistic studies. Kinetic monitoring highlighted the critical role of the soluble base and clarified aspects of the reaction pathway towards selective oxidation. Moreover, the study demonstrates that quasi-homogeneous Pd nanocatalyst combines high efficiency and selectivity with minimal material use, making a promising system for sustainable bio-sourced chemical production. These findings lay the groundwork for optimization of catalytic processes, offering new perspectives for designing stable and environmentally benign catalysts for HMF valorization.

¹ Zhang, Z.; Deng, K.; *ACS Catal.* 2015, 5, 11

² Lai, J.; Zhou, S.; Cheng, F.; Guo, D.; Liu, X.; Xu, Q.; Yin, D.; *Catal. Lett.* 2020, 150, 1301

³ Bourbiaux, D.; Mangematin, S.; Djakovitch, L.; Rataboul, F. *Catal. Lett.* 2021, 151, 3239

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The word "FLASH" is written in a bold, white, sans-serif font. It is centered within a dark green rectangular box that has a slightly textured or distressed appearance.

FLASH

Synthesis of C-glycosides derivatives by mechanosynthesis

Pauline FRAMBOURG, Solen JOSSE, Anne WADOUACHI

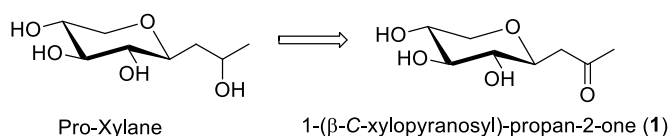
Laboratoire LG2A (Laboratoire de Glycochimie et des Agroressources d'Amiens), UR 7378,

10 Rue Baudelocque, 80000 Amiens

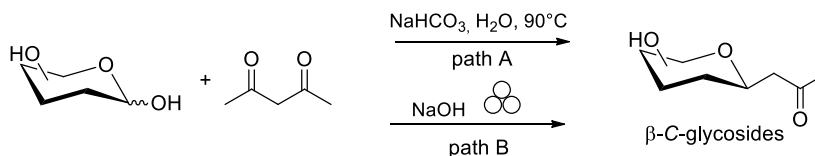
pauline.frambourg@etud.u-picardie.fr

The climate challenges we face are leading us to rethink our synthesis methods and adopt a more environmentally friendly approach, proposing strategies that best follow the principles of green chemistry. This project is part of this approach, proposing mechanochemical synthesis of β -C-glycosides derivatives from free sugars and diketones.

These compounds are of interest to the cosmetics and pharmaceutical industries. For example, Pro-Xylane® is a C-glycoside with anti-aging properties that is obtained by reducing 1-(β -C-xylopyranosyl)-propan-2-one (1).



The reaction of a free sugar in the presence of penta-2,5-dione in alkaline solution was developed by Lubineau et al (path A).¹ We have developed the synthesis of these β -C-glycosides derivatives by mechanochemistry using a stoichiometric amount of diketone and water only as LAG (path B).²



Following on from this work, we focused on expanding access to various β -C-glycosides derivatives through mechanochemistry.



The results presented here will focus on the development of synthesis from different diketones with optimisation of grinding parameters.

¹ Rodrigues, F.; Canac, Y.; Lubineau, A. *Chemical Communications* **2000**, 2049

² J. Thiel, I. Malpartida, V. Lair, S. Halloumi, F. Lacoste, A. Wadouachi, S. Josse, E. Beaupparain WO 2025/01462 A1, **2025**

TOWARD A CHEMOSELECTIVE AMIDE-TO-AMINE REDUCTION VIA MECHANOCHEMISTRY FOR THE SYNTHESIS OF UNNATURAL AMINO ACIDS

Hidalgo Anatole, Schneider Séverine, Bihel Frédéric*

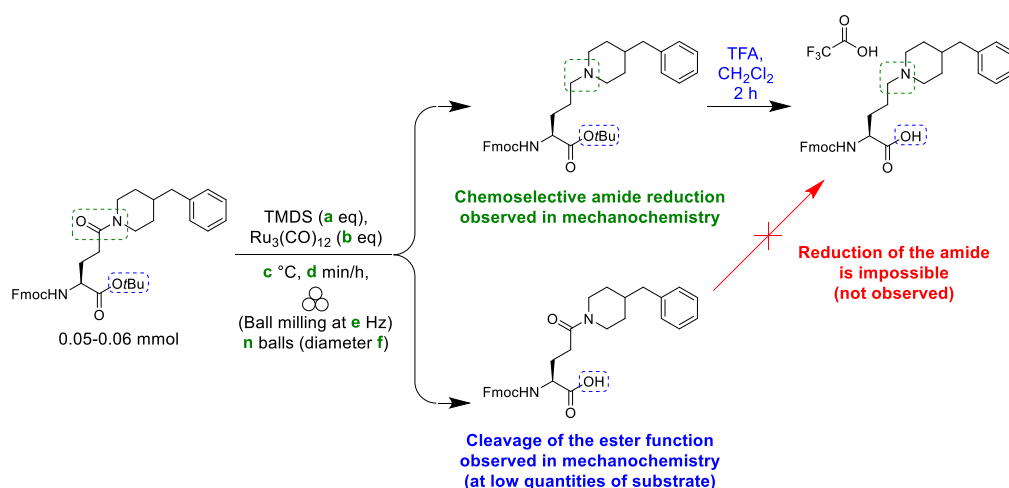
Université de Strasbourg, Laboratoire d'Innovation Thérapeutique, CNRS/Unistra UMR7200

*fbihel@unistra.fr

Chemical processes often entail the use of solvents, which can pose environmental concerns because of their toxicity, non-sustainable sourcing and significant contribution to waste generation, with solvents accounting for nearly 80% of reaction by-products¹. To address these issues, mechanochemistry has emerged as an effective solvent-free method, with an increasing amount of synthesis of active pharmaceutical ingredients being reported in the literature².

The objective of this work was to achieve the mechanochemical ruthenium-catalyzed chemoselective reduction of a tertiary amide to an amine, a key step in the synthesis of unnatural amino acids N-Fmoc-AA-OH bearing a tertiary amine on their side chain. These amino acids are of particular interest as ready-to-use building blocks for solid phase peptide synthesis³.

An HPLC-based analytical method was developed to quantify conversion and yields. However, under the tested conditions, degradation of the products was observed, particularly at the OtBu ester protecting group. Attempts to perform the reduction from the corresponding carboxylic acid proved unsuccessful. Further investigations revealed that degradation of the ester functionality was primarily due to the low substrate loading.



¹ Kerton, F. *Alternative Solvents for Green Chemistry*; 2009; pp 1–22.

² Bento, O. *et al. Eur. J. Org. Chem.* **2022**, 2022 (21), 109.

³ Schneider, S. *et al. Org. Biomol. Chem.* **2015**, 13 (25), 7020.

NANOCOMPOSITES OF BIOCHAR AND TITANIUM DIOXIDE NANOTUBES FOR DYE DEGRADATION UNDER UVC LIGHT

Emma Demathieu¹, Tâm Thị Bằng Đào², Chí Nhân Hà Thúc^{2*}

¹ Univ. Savoie Mont Blanc, Master Chimie Verte et Eco-Innovations, UFR Science et Montagne

² Vietnam National University – Ho Chi Minh City, Univ. of Science, Faculty of Materials Science and Technology
emma.demathieu@etu.univ-smb.fr

Industrial wastewater, particularly from textile industries, often contains persistent organic dyes that are harmful to both human health and the environment. Conventional treatment methods are often insufficient for complete degradation, creating a pressing need for sustainable and efficient alternatives, particularly in developing countries such as Vietnam, where textile activity is intense and wastewater pollution remains a major environmental challenge.

This study was carried out during an internship at a Vietnamese research institute, focusing on photocatalysis as a promising advanced oxidation process capable of generating reactive oxygen species to degrade resistant organic pollutants.

Biochar/TiO₂ nanocomposites were synthesized for photocatalytic dye degradation under UVC light. The adsorbent phase, derived from rice husk ash, makes use of an abundant local agricultural waste, while the photocatalytic phase, composed of titanium dioxide nanotubes obtained by hydrothermal treatment, ensures high semiconducting efficiency.

Several nanomaterials with varying biochar/TiO₂ ratios were tested for adsorption and photocatalytic degradation of Basic Blue 3 dye. Results showed that the richer the nanocomposite is in biochar, the higher its adsorption capacity will be. Unfortunately, the adsorption capacity of the synthesized biochar was insufficient to improve degradation during photocatalysis. This was demonstrated in the degradation tests where, despite the combination of both properties in nanomaterials, titanium dioxide nanotubes alone exhibited more efficient dye degradation than the nanocomposites.

Future work will therefore focus on the development of activated carbon-based composites to further improve adsorption efficiency and so overall photocatalytic performance.

This study highlights the potential of combining waste-derived materials with nanostructured photocatalysts for sustainable wastewater treatment applications.

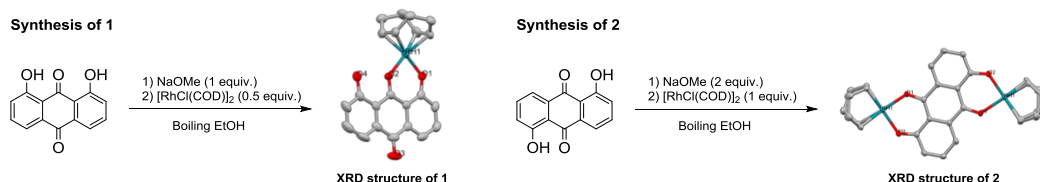
PHOTOACTIVE COMPLEXES FOR CARBONYLATIVE PROCESSES

Hossam Farouk, Loris Geminiani, Daniel Pla*, Montserrat Gómez*

*Fundamental and Applied Heterochemistry Laboratory, University of Toulouse, France
hossam.ahmed-farouk-abdelmaksoud@utoulouse.fr*

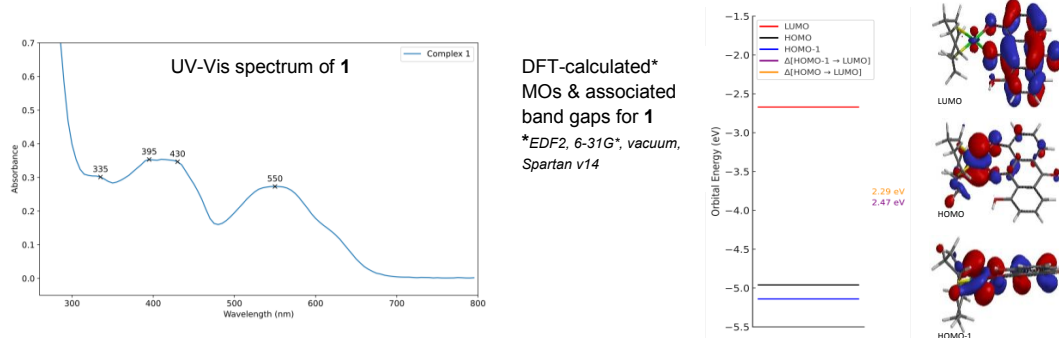
Hydroaminomethylation (HAM) represents an efficient and selective route for the synthesis of amines through a one-pot multicomponent transformation, involving the activation of carbon monoxide and hydrogen.¹ Recent studies of our group proved that Rh/Co-based cooperative catalytic systems enhanced the rate-limiting enamine hydrogenation step, using glycerol as solvent under thermal conditions.^{2,3,4}

Herein, we describe the synthesis of mono- and bimetallic complexes bearing UV-Vis active dihydroxyanthraquinone ligands (1,5-DHAQ and 1,8-DHAQ) to elucidate plausible cooperative effects. Thus, $[\text{Rh}(\eta^2\text{-1,8-DHAQ-H})(\text{COD})]$ (**1**) and $[\text{Rh}_2(\mu^2, \eta^2\text{-1,5-DHAQ-2H})(\text{COD})_2]$ (**2**) were isolated and fully characterized (NMR, UV-Vis, FT-IR, HRMS, single-crystal XRD).



DFT calculations provided HOMO-LUMO energy gaps in close agreement with the UV-Vis absorption profiles, supporting the potential of DHAQ-based systems for future photo-activated carbonylative catalysis.

Preliminary catalytic tests using complex **1**, proved the selectivity of the multi-step HAM process towards the enamine formation, precluding its further hydrogenation.



¹Kalck, P.; Urrutigoñy, M. Tandem Hydroaminomethylation Reaction to Synthesize Amines from Alkenes. *Chem. Rev.* **2018**, 118 (7), 3833–3861.

²Pérez Alonso, A.; Pham Minh, D.; Pla, D.; Gómez, M. A Cooperative Rh/Co-Catalyzed Hydroaminomethylation Reaction for the Synthesis of Terpene Amines. *ChemCatChem* **2023**, 15.

³Pérez Alonso, A.; Gibot, L.; Favier, I.; Pham Minh, D.; Gómez, M.; Pla, D. Antiproliferative in Vitro Evaluation of Terpenic Amines Synthesized via a Rhodium-Catalyzed Hydroaminomethylation. *Chem. Biodivers.* **2024**.

⁴Serrano-Maldonado, A.; Dang-Bao, T.; Favier, I.; Guerrero-Ríos, I.; Pla, D.; Gómez, M. Glycerol Boosted Rh-Catalyzed Hydroaminomethylation Reaction: A Mechanistic Insight. *Chem. Eur. J.* **2020**, 26, 12553.

EXPLORING CeNi₅ AS A NEXT-GENERATION CATALYST FOR SUSTAINABLE HYDROGEN PRODUCTION BY DRY REFORMING OF METHANE

M. Moreau¹, G. Garbarino², R. Freccero³, P. Riani³

1: IC2MP, University of Poitiers, B27, TSA 51106, 4 rue M. Brunet 86073 Poitiers cedex 9

2: DICCA – Dipartimento di Ingegneria Civile, Chimica e Ambientale, Università degli Studi di Genova, Via all'opera Pia 15, 16145 Genova, Italy

3: DCCI - Dipartimento di Chimica e Chimica Industriale, Università degli Studi di Genova, Via Dodecaneso 31, Genova

Mila.moreau@etu.univ-poitiers.fr

As part of the European Union's new environmental regulations, reducing greenhouse gas emission, particularly carbon dioxide (CO₂), is essential to achieve climate neutrality by 2050. Emissions must decrease by 55% by 2030, prompting intense research on both emission reduction and CO₂ valorization. Unlike other greenhouse gases such as methane (CH₄) or nitrous oxide (N₂O), CO₂ persists in the atmosphere, exerting a long-term cumulative effect. Among the available conversion routes, dry reforming of methane (DRM) simultaneously consumes methane (CH₄) and CO₂ while producing syngas (CO and H₂). Catalysts for CO₂ methanation must exhibit high activity and selectivity, as well as resistance to deactivation, to produce methane at low temperatures. Therefore, transition metals like nickel offer a good balance between activity and cost. To further provide better characteristics such as metal dispersion, deactivation resistance, or carbon dioxide absorption capacity, some studies have focused on the use of bimetallic catalysts, in which the second metal acts as a promoter. Such qualities are currently being investigated with lanthanides, which modify electronic and textural properties through redox behavior and oxygen defect generation. In this context, CeNi₅ emerges as a promising bimetallic catalyst for DRM. Catalytic tests demonstrated that the CeNi₅-based catalyst exhibits promising activity for DRM, showing good CO₂ and CH₄ conversion rates and stable H₂ and CO production at high temperatures, achieving peak activity at 1073 K. However, carbon deposition was observed post-reaction, requiring further attention, possibly through regeneration strategies or catalyst modification.

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POSTERS

Amine-functionalized polymers as materials to CO₂ capture

Masheer UL HAQ, Jean-Daniel Marty, Christophe Coudret, Nancy Lauth-de Viguerie

Université de Toulouse
Laboratoire SOFTMAT, UMR-CNRS 5623
nancy.de-viguerie@utoulouse.fr

The CONFETI project (Green valorisation of CO₂ and Nitrogen compounds for making FERTIlizers), funded by the EU EIC Pathfinder program, aims to develop a lab-scale autonomous technology capable of capturing and photo-electrochemically converting CO₂ and nitrogen directly from air or flue gases into urea, produced and delivered in situ using renewable energy sources.¹

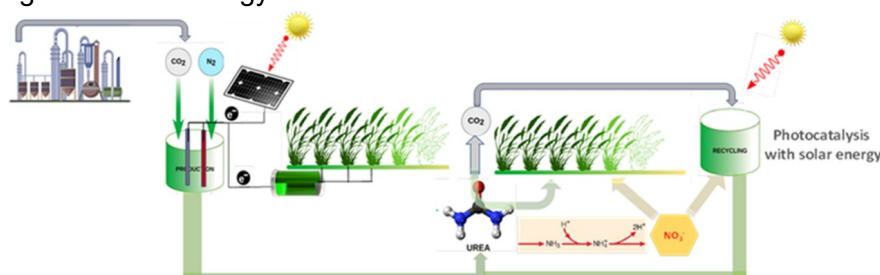


Fig. 1. CONFETI approach to lab-scale production of urea from N (N₂ and/or NO₃⁻) and CO₂.

A major challenge in the project is designing materials that efficiently capture and release CO₂ for subsequent electrochemical conversion into urea. To address this, we investigated composite membranes combining amine-functionalized polymers, such as branched polyethyleneimine, poly(N-vinylamine), and poly[N-[2-(diethylamino)ethyl]acrylamide], with ionic liquids (EMIMTFSI, BMIMBF₄). These composites are designed to have strong chemical affinity for CO₂ with enhanced gas diffusivity. Chemical crosslinking strategies were applied to produce self-standing, mechanically robust membranes suitable for gas-diffusion electrochemical cells.

The monitoring of CO₂ capture was central to the selection process. For this purpose, we used the Quartz Crystal Microbalance with Dissipation (QCM-D) technique to follow adsorption and desorption in real time.² CO₂ adsorption was performed under a CO₂ flow, and desorption under a N₂ flow, enabling evaluation of how amine type, film thickness, and cross-linker content influence both CO₂ uptake and release behavior.

This work provides key insights for the ongoing development of CO₂-responsive membranes for potential integration into the gas-diffusion electrochemical reactor of the CONFETI project.

¹ Chen Chen *et al.*, *Nature Chemistry* (2020), **12**, 717–724

² John R Hoffman, Avery E Baumann, Christopher M Stafford, *Chem Eng J.* (2024), **481**, 148381

ARE ALL BIOBASED MATERIALS SUSTAINABLE?

Marion ROULLET, Laure BINIEK

Atelier CIRCULR, L'Exploratorium, Afpa Strasbourg, Rue des Corps-de-Garde, Strasbourg
marion.roullet@ateliercirculr.fr et laure.binieck@ics-cnrs.unistra.fr

Biobased materials and chemicals appear as a promising solution to mitigate climate change, by reducing the use of fossil resources and the related greenhouse gases emissions. However, a mere substitution of fossil resources with natural resources for chemistry, at the same production rate, and in a linear and capitalistic economy, would accelerate the damage to the other planetary boundaries. Indeed, climate change is only one aspect of the environmental crisis, as it is interconnected with the decline of biodiversity, the accumulation of pollutions, the jeopardised soil health and the disrupted geo-chemical cycles. Solving the ecological crisis, in a spirit of social justice, requires not only technological changes, but also radical societal transformations¹.

It is thus essential to embrace the material transition with a systemic approach, coupling technological innovation with social innovation. This involves questioning our practices of research and development.

In this presentation, the development of materials for a sustainable, fair and empowering society will be used as a case study for an holistic approach of responsible research. Coming back to biobased materials, this approach invites to extend the criteria to include the restriction to agrifood by-products as resources, biodegradability, a business model for the production that puts sufficiency at its core, and the anchoring of the materials in their territory by involving all the stakeholders from the research stage. Heat-pressing will be used as an example of promising "low-tech" material processing².

This versatile and technique transforms food & drink byproducts (e.g. spent tea leaves, spent brewers grains, apple pomace, sheep wool) into rigid biodegradable materials, either as boards or molded objects. The association Atelier CirculR makes this technique accessible to designers, researchers and craftsmen, in its third place, l'Exploratorium. The objective is to anchor this technique in the territory, by practicing citizen science and finding applications that correspond to the local needs.

¹Fanning, A. L.; Raworth, K. Doughnut of Social and Planetary Boundaries Monitors a World out of Balance. *Nature* **2025**, 646 (8083), 47–56. <https://doi.org/10.1038/s41586-025-09385-1>.

² Jumeaux, M.; Touchaleaume, F.; Durrieu, V.; Vandebossche, V.; Vaca-Medina, G.; Rouilly, A. Melt Processing of Unrefined Horn Keratin. *ACS Sustainable Chem. Eng.* **2023**, 11 (42), 15423–15431. <https://doi.org/10.1021/acssuschemeng.3c04502>.

DEEP EUTECTIC SOLVENTS AS MEDIA FOR COVALENT ORGANIC FRAMEWORKS SYNTHESIS

Pauline André^a, Alex-Gabriel Marina^a, Michaël Teixeira^a, Francesca Maria Faroni^a, Benoît Louis^b and Stéphane Baudron^a

^a Université de Strasbourg, CNRS, CMC UMR 7140
Equipe Synthèse et Fonctions des Architectures Moléculaires

^b Université de Strasbourg, CNRS, ICPEES, UMR 7515

e-mail : pauline.andre@etu.unistra.fr

Covalent organic frameworks (COFs) are bi- or tridimensional porous polymers formed through covalent bonds between organic building blocks. With high surface areas and remarkable chemical and thermal stability, COFs have promising applications in drug delivery, gas sorption, and catalysis.¹ Conventional synthesis relies on toxic solvents such as mesitylene and dioxane, requiring prolonged reaction times at high temperatures. To develop a more sustainable alternative, one can consider the use of deep eutectic solvents (DESs).² DESs are mixtures of at least two components which, at the eutectic ratio, feature a depression of the melting point. Those solvents are easily prepared, cheap, less toxic and biodegradable, making them interesting media for COF synthesis.³

In this context, our research focuses on the synthesis of imine based bidimensional COFs, using DESs, such as choline chloride : acetic acid (1:2), as alternative synthetic media (Figure 1). In this contribution, our first results will be presented showing reduction of heating time and temperature, significantly lowering energy consumption and the environmental impact. Furthermore, influence of DES synthesis on COF properties such as crystal morphology and sorption behavior will also be highlighted.

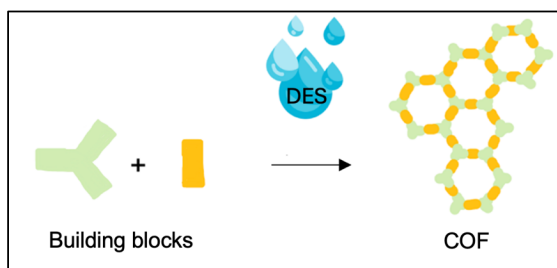


Figure 1. The use of deep eutectic solvents for the synthesis of covalent organic frameworks

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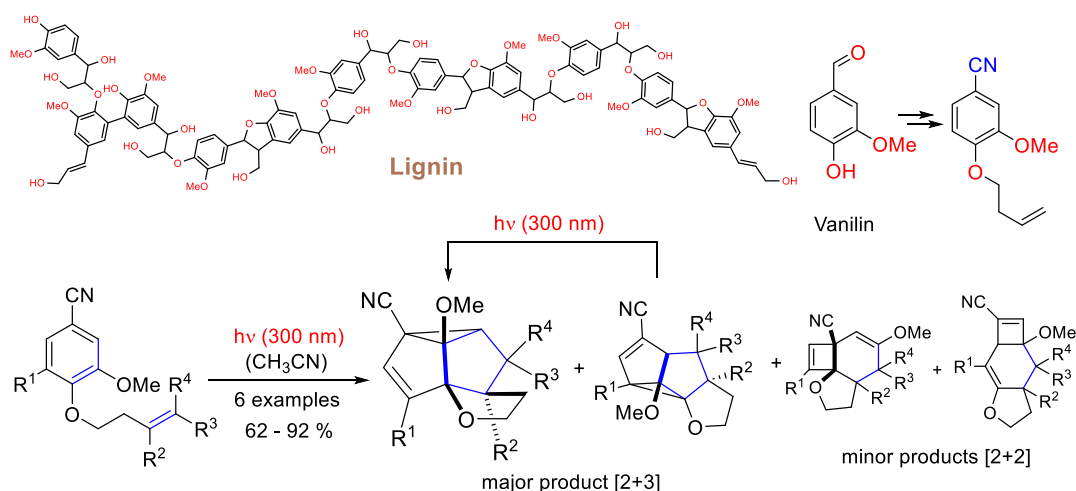
PHOTOCYCLOADDITIONS WITH LIGNIN DERIVED AROMATIC COMPOUNDS

Norbert Hoffmann, Arthur Desvals

CNRS, Université de Strasbourg, IPCMS (UMR 7504), 23 rue du Loess, 67034 Strasbourg, France. norbert.hoffmann@ipcms.unistra.fr

Lignin is an important component of biomass. In connection with the chemical utilization of this renewable raw material, lignin is the main source of aromatic compounds.¹ For example, vanillin is produced from lignin on the industrial scale.² In the context of sustainable chemistry, we are particularly interested in intramolecular photocycloadditions with such derivatives (Scheme). Starting from simple structures, a high degree of molecular diversity and complexity is generated in only one step.³ The formation of new C-C bonds occurs without chemical activation. No acids, no bases, or catalysts are needed, which reduces the formation of waste products. The photon is considered as a traceless reagent.⁴

We are also interested in studies of the reaction mechanism in order to optimize the reaction conditions. The competition between the formation of the main products (resulting from a [2+3] cycloaddition) and the formation of the minor products (resulting from a [2+2] cycloaddition) depends on the substitution pattern at the reaction centers. The spin multiplicity of the excited state also plays a decisive role in this competition.



Scheme. Intramolecular photocycloadditions with lignin derived aromatic compounds.

¹ Argyropoulos, D. D. S.; Crestini, C.; Dahlstrand, C.; Furusjö, E.; Gioia, C.; Jedvert, K.; Henriksson, G.; Hultberg, C.; Lawoko, M.; Pierrou, C.; Samec, J. S. M.; Subbotina, E.; Wallmo, H.; Wimby, M. *ChemSusChem* **2023**, *16*, e202300492. <https://doi.org/10.1002/cssc.202300492>

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Upcycling Biomass into Bright Graphene Quantum Dots for Sensing and Photocatalysis

Philippe Pierrat

Université de Lorraine, CNRS, L2CM, UMR7053, B.P 95823, 57078 Metz, France

philippe.pierrat@univ-lorraine.fr

Graphene quantum dots (GQDs) are emerging as a highly promising class of 2D carbon-based nanomaterials, offering a compelling alternative to traditional organic dyes and heavy metal-based quantum dots. Their exceptional properties (chemical stability, low photobleaching, tunable photoluminescence, and low cytotoxicity) make them attractive for a wide range of applications, from biosensing to energy storage.^{1,2}

However, the scalability and high production costs of GQDs remain significant barriers to their broader industrial adoption. In response to this challenge, we have developed a rapid, efficient, and reproducible method to produce tens of grams of GQDs from non-food biomass wastes (e.g., banana and vegetable peels). This sustainable, high-yield process, performed under microwave irradiation, offers a cost-effective route to high-quality GQDs.

The resulting water-soluble nanoparticles exhibit excitation-dependent luminescence, shifting from blue to orange in solution. Remarkably, solid-state films of pure GQDs emit white light under UV excitation, an uncommon and valuable feature that bypasses the typical aggregation-induced quenching and opens up exciting opportunities in optoelectronics.³

Beyond their optical properties, these GQDs function as sensitive and selective fluorescence sensors for metal cations such as Hg^{2+} , Fe^{3+} , and Sn^{2+} , with competitive detection limits. High-resolution TEM reveals the *in-situ* formation of coordination networks upon metal binding, highlighting their potential in catalyst design. Furthermore, we have demonstrated their versatility as green photocatalysts, capable of degrading organic pollutants (e.g., rhodamine, ciprofloxacin) and generating hydrogen from water under light irradiation.

Altogether, our work positions biomass-derived GQDs as sustainable, multifunctional nanomaterials with significant promise for advanced sensing, catalysis, and energy applications.

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Comparative phytochemical study and bio-activity activities of pure and nano-encapsulated essential oil in liposome (lecithin) from Djiboutian *Cymbopogon commutatus* and three commercial *Cymbopogon*

ABDIRAHMAN ELMI^{1*}, **ROSELLA SPINA**², **FATOUMA M. ABDOUL-LATIF**¹,
ANDREEA PASC³, **ARNAUD RISLER**³, **STEPANIE PHILIPPOT**³, **RAPHAEL DUVAL**³, **DOMINIQUE LAURAIN MATTAR**²

¹ Centre d'Etudes et de Recherche de Djibouti, Medicinal Research Institute, IRM-CERD, Route de l'Aéroport, Haramous B.P. 486, Djibouti City, Djibouti;

² Université de Lorraine, INRAE, LAE, F-54000 Nancy, France;

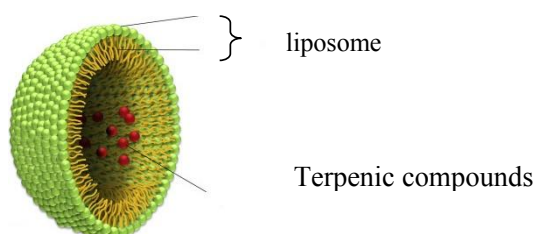
³ Université de Lorraine, CNRS, L2CM, F-54000 Nancy, France ;

Abstract:

In our previous research, we discovered that essential oils (EOs) from the *Cymbopogon* genus, known locally as Caws Dameer or Dambahu, have significant anti-cancer properties. We analyzed EOs from four *Cymbopogon* species using GC-MS and found a significant variation in their phytochemical composition. Oxygenated monoterpenes were the dominant components in all species, with (+)-(R)-Limonene, geraniol, and alpha- and gamma-elemene being the most common compounds across the species.

However, the primary terpene components of these essential oils are delicate and have low water solubility, which limits their effectiveness. To overcome this, we developed a method to encapsulate these compounds using naturally derived polymeric matrices, specifically soybean lecithin. This approach aims to improve the preservation and bioavailability of these essential oils.

The resulting nano-emulsions have demonstrated enhanced biological activity, decreased toxicity, and improved homogenization in aqueous mediums. However, their stability under normal conditions needs to be improved.



Nanoemulsion system, Afornali et al. 2016/ modified

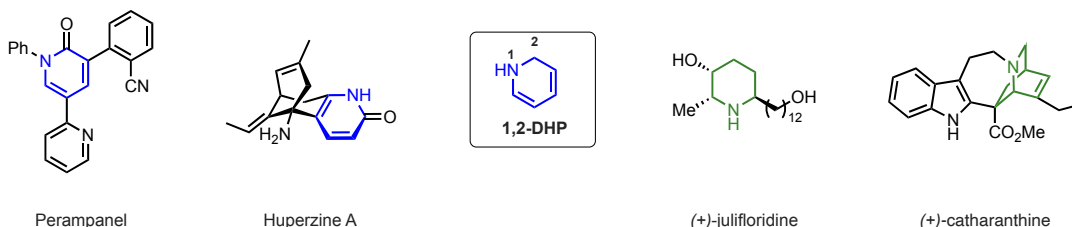
Development of new methods for the synthesis of nitrogen-containing heterocycles catalyzed by gold(I)-polyoxometalates complexes

Titien SIMON, Stefan CHASSAING and Aurélien BLANC.*

University of Strasbourg, Laboratoire de Chimie Organométallique, Synthèse organique et Santé : COSyS UMR 7177, 4 rue Blaise Pascal, 67000 Strasbourg.

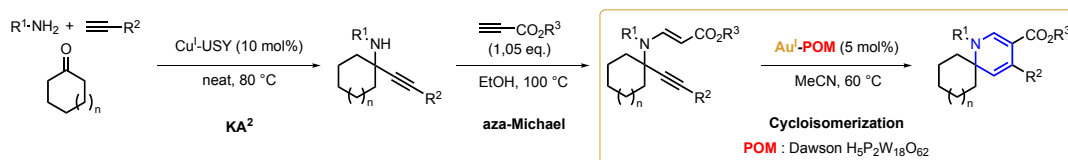
titien.simon@etu.unistra.fr

Nitrogen-containing heterocycles have always attracted considerable interest in organic synthesis and medicinal chemistry due to their wide range of biological activities. Currently, approximately 60 % of drugs are based on nitrogen-containing heterocycles, highlighting their importance in the design of new drugs.¹ Among these structures, **1,2-dihydropyridines**, although rare, exhibit interesting biological activities, notably on the nervous system.² These molecules also serve as key intermediates in synthesizing **piperidines** and **isoquinuclidines**, scaffolds found in natural alkaloids.³ (Scheme 1).



Scheme 1

Therefore, accessing the **1,2-dihydropyridine** framework has been the subject of significant research. Among the various approaches reported, the cycloisomerization of aza-1,5-enynes has emerged as an attractive tool due to its excellent atom economy. In our laboratory, we developed a route to highly functionalized **spiro-1,2-dihydropyridines** using heterogeneous copper(I)-doped zeolite catalysis (Cu^I-USY Ultra-Stable Y).⁴ To address the limitations of the zeolite-catalyzed version, this project proposes using gold(I)-based heterogeneous catalysts supported on **polyoxometalates** (POMs).⁵ In addition to being generally inexpensive, easy to prepare, and straightforward to recover/recycle, our supported catalysts have proven highly efficient for various significant organic transformations, allowing access to key molecular "building blocks" for the chemical and pharmaceutical industries under "green" conditions.



Scheme 2

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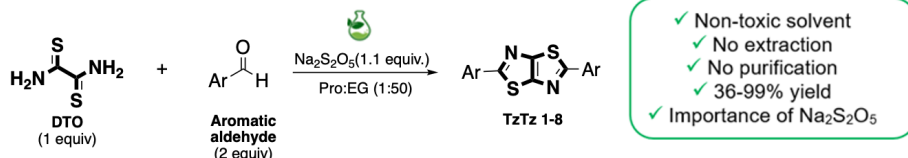
ECO-FRIENDLY SYNTHESIS OF THIAZOLO[5,4-D]THIAZOLES AND THEIR DERIVATIVES BEARING AZOLES UNITS

Thien Thuy Trang Nguyen¹, Jean-François Longevial¹, Stéphanie Hesse¹

¹ LCP-A2MC, Université de Lorraine, 1 Bd Arago, 57070 Metz, France
thien-thuy-trang.nguyen@univ-lorraine.fr

Thiazolo[5,4-*d*]thiazoles (TzTz) are a class of heteroaromatic compounds that have attracted increasing interest in the fields of organic synthesis, electronics, and biology, due to their π -conjugated systems and their rigid planar backbones.¹ To date, most synthetic routes toward TzTz derivatives are still based on the classical method developed by Ketcham *et al*², which involves a double condensation between dithiooxamide and suitable aldehydes and then oxidation of the intermediate product. However, this approach usually requires harsh reaction conditions, toxic solvents, and troublesome isolation and purification steps.³

This study aims to develop a greener and more environmentally friendly synthetic protocol using deep eutectic solvents (DES) to enable a straightforward access to TzTz derivatives without further purification. By optimizing the reaction parameters by modifying the nature and ratio of DES components, changing the activation method, and adding auxiliary oxidants, eight TzTz derivatives were synthesized in equal or better yields compared to the reported protocols (ranging from 20% to 75%) under mild and eco-friendly conditions, in L-proline and ethylene glycol (1:50) mixture, with the presence of sodium metabisulfite as oxidant, at 130 °C for one hour.⁴



In a further effort to enhance π -conjugation and introduce new functionalities, this work also explored the functionalization of the TzTz scaffold at the 2,5-positions with azole units such as imidazole, benzimidazole, and triazole via two different synthetic strategies. Among them, nucleophilic aromatic substitution ($\text{S}_{\text{N}}\text{Ar}$) between azole amines and bis(4-fluorophenyl)-substituted TzTz emerged as a promising method to diversify the TzTz core. Preliminary photophysical characterizations revealed that these TzTz bearing azoles derivatives exhibit notable absorption and fluorescence behavior, underlining their potential as building blocks for organic optoelectronic application.

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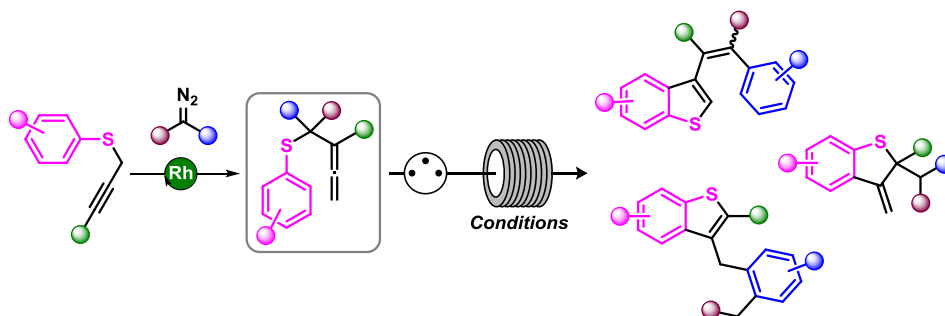
DIVERSITY-ORIENTED TRANSFORMATION OF DOYLE-KIRMSE PRODUCTS

Timothé Maujean, Camille Van Wesemael, Patrick Wagner, Mihaela Gulea, Romain Pertschi

Faculté de Pharmacie, Université de Strasbourg, 74 route du Rhin, 67400 Illkirch, France
maujean@unistra.fr

Diversity-Oriented Synthesis¹ (DOS) and cascade rearrangement reactions represent powerful strategies that, when combined, can significantly accelerate drug discovery by providing a rapid access to a large variety of complex compounds from simple precursors. The Doyle-Kirmse [2,3]-sigmatropic rearrangement represents a good example of such a strategy, yielding complex compounds with various points of diversification starting from readily available thioethers and diazo compounds.² However, despite the high interest for this reaction only few post-Doyle-Kirmse reactions have been developed, especially when an allene is obtained as the [2,3] rearrangement product.³

In this context, a modular and divergent approach toward thiophene-derived structures has been developed using flow chemistry involving cascade reactions starting from a unique precursor, obtained through a rhodium-catalysed rearrangement (Scheme 1). The corresponding allenes were heated at high temperatures in *tert*-amyl alcohol to trigger multiple cascade sequences yielding three different benzothiophene derivatives, depending on the conditions used and substrate structures. Overall, this strategy allowed a swift and direct access to complex molecular structures containing S-heterocyclic scaffolds of interest in drug discovery.⁴



Scheme 1

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In vitro* antifungal effect of essential oils and *in silico* identification of highly potent natural fungicides against *Alternaria alternata

Khaoula Chattat^{*1,2}, Amal SAMMAMA², Rachid AZENZEM, Abderramane FARAGI^{1,3}, Tayeb KOUSSA¹, Mohamed Najib ALFEDDY²

¹ Laboratory of Plant Biotechnology, Ecology and Ecosystem Valorization, URL - CNRST N°10, Faculty of Sciences, Chouaib Doukkali University, Av. Jabrane Khalil Jabrane, B.P. 299, 24000 El Jadida, Morocco

² Plant Protection Research Unit, Regional Center of Agricultural Research of Marrakech, National Institute of Agricultural Research, Avenue Ennasr, BP 415 Rabat Principale, 10090 Rabat, Morocco

³ Laboratory of Agri-food and Health, Faculty of Science and Technology, Hassan Frist University, University Complex, Casablanca Road, BP. 577, 26000 Settat, Morocco
**chattat.khaoula@ucd.ac.ma*

Abstract

Olive leaf spot disease, caused by the fungus *Alternaria alternata*, poses a severe threat to olive production. Concerns regarding fungicide resistance and its environmental impact have generated significant interest in developing alternatives to chemicals. In this direct, essential oils can undoubtedly perform a fundamental role. Therefore, this study aims to study the antifungal activity of some essential oils extracted from aromatic and medicinal plants in individual and combined forms against olive leaf disease caused by *Alternaria alternata*. The chemical composition of the studied essential oils was identified by GC-MS. Moreover, the antifungal activity was investigated. All the essential oils tested showed significant antifungal activity against the fungi studied. These findings suggest a new research avenue for essential oils to be expanded as novel natural formulations useful in agriculture as ecologically sustainable, reliable, and socially acceptable alternatives to fungicides. In addition, the affinity of highly potent natural compounds of essential oils was studied against a key enzyme involved in the *Alternaria alternata* infection process, using advanced molecular dynamics techniques. A list of plant metabolites with antifungal properties was compiled for evaluation as potential fungicides. The results revealed stable interactions between the selected metabolites and the target proteins. The SwissADME server analysis indicated that the metabolites possess fungicide properties, making them effective and safe fungicides with low toxicity to the environment and living beings. Furthermore, bioactivity assays confirmed their biological. These results are of great significance and provide a solid basis for the development of strategies to protect the olive trees.

Keywords: Antifungal, chemical compounds, foliar disease, molecular docking, *Olea europaea*

NITROGEN-ENRICHED ACTIVATED CARBONS FOR THE CAPTURE AND SEPARATION OF CO₂

Kouassi F. N'GOLE ^{1,2*}, Rafael MORALES-OSPINO ², Laurence REINERT ¹, Bernard DAVID ¹, Vincent NICOLAS ², Jimmy NICOLLE ³, Fatou CONDÉ ³, Alain CELZARD ^{2,4}, Vanessa FIERRO ¹, Laurent DUCLAUX ¹

¹ Université Savoie Mont Blanc, CNRS, EDYTEM, 73000, Chambéry, France

² IJL, Université de Lorraine, CNRS, F-88000, Epinal, France

³ ICMN, CNRS/Université d'Orléans, 1B rue de la Férollerie, 45071 Orléans cedex, France

⁴ Institut Universitaire de France (IUF), 75231 Paris, France

[*Kouassi-fabrice.n-gole@univ-smb.fr](mailto:Kouassi-fabrice.n-gole@univ-smb.fr)

Keywords: adsorption; CO₂ capture; activated carbons; CO₂ separation.

As carbon dioxide (CO₂) is one of the main greenhouse gases, the increase in its concentration in the atmosphere leads to global warming. For this reason, numerous researches are presently focused on CO₂ separation from industrial gases in the post-combustion process. In this work, nitrogen-enriched Activated Carbons (ACs) with nitrogen content up to 10 wt.% were synthesized in two successive steps in the same furnace: (i) pyrolysis (10K.min⁻¹, 1173K, N₂, 200 mL.min⁻¹) of nitrogen-rich precursors: powder and lyophilized chitosan beads (7 wt.% N), coffee grounds (3 wt.% N) and polyacrylonitrile powder (26 wt.% N) and (ii) ammonia gasification activation at 1173K (NH₃ flow: 30-36 mg.min⁻¹, activation time: 15-120 min). The physisorption isotherms at 77K of N₂ and H₂ indicated that the synthesized ACs are mainly microporous, and the BET areas are in the range from 325 to 1390 m².g⁻¹. Adsorption capacities of ACs were studied at three different temperatures 273K, 298K and 323K. The amount of CO₂ physisorbed at 1 bar ranged from 1.79 to 2.98 mmol/g at 298K. The calculated isosteric adsorption heat shows stronger interactions between CO₂ and the surface groups of ACs (22.07-31.18 kJ.mol⁻¹ at 1 bar), and weak interactions between N₂ and the surface groups of ACs (10.35-20.04 kJ.mol⁻¹ at 1 bar). To assess the ability of ACs to select CO₂ over N₂, the CO₂/N₂ selectivity (15% vol. of CO₂) was calculated using the pure gases' adsorption isotherms and the Ideal Adsorbed Solution Theory (IAST) model. At 298K, CO₂/N₂ selectivity reaches values between 24 and 110. ACs from coffee grounds activated for 60, 90 and 120 min exhibit higher selectivity attributed to the optimal balance between textural properties and surface groups. To better understand this behavior at 298K, Principal Component Analysis (PCA) and Partial Least Squares regression (PLS regression), statistical methods were used. They showed that the ultra-micropore volume, the amount of CO₂ adsorbed, and the impurities present in ACs influence the CO₂/N₂ selectivity at 298K. Furthermore, energy dispersive X-ray spectroscopy showed that the impurities likely to influence selectivity at T>298K could be minerals containing Mg, P, Ca, and K.

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POLYMERS SOFT TEMPLATES FOR SYNTHESIS OF CATALYTIC MATERIALS

Lucia Turazza, Elisa Leonard,
Barbara Lonetti* and Eliza-Diana Ciuculescu-Pradines*
barbara.lonetti@utoulouse.fr; eliza.ciuculescu-pradines@utoulouse.fr

Université de Toulouse, Laboratoire SoftMat- Chimie des colloïdes, polymères & complexes
(Bat 2R1 recherche de Chimie, 118 Route de Narbonne 31062 Toulouse cedex 4 – France)

Amphiphilic block copolymers (BCPs), consisting of a hydrophilic and a hydrophobic segment, have attracted significant attention due to their ability to self-assemble into nanoscale ordered structures.¹ Especially, reverse or type II morphologies such as cubosomes and hexosomes structures are formed, when the interface curves toward the hydrophilic domain facilitating a negative curvature.² These polymer-based structures are particularly appealing in nanotechnology and materials science because of their high loading capacities, as well as their exceptionally large specific surface areas. Therefore, these structures can be used as soft templates for synthesizing various mesoporous functional materials.³ The template can be removed post-synthesis, yielding materials with high porosity and surface area.

In this study, we present preliminary findings using a PLA_{29k}-*b*-PEO_{2k} block copolymer that forms hexosomes. These structures were successfully loaded with organic ligands such as polyphenols (e.g., gallic acid) without compromising their integrity. This opens up promising avenues for incorporating metal ions such as Fe, capable of complexing with gallic acid. The samples were characterized using SAXS and SEM techniques.

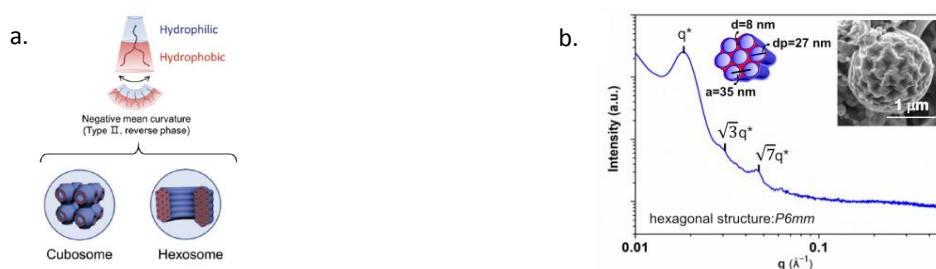


Figure 1: a. Type II self-assembly of BCPs in solution. b. SAXS profile of *P6mm* Hex of PLA_{29k}-*b*-PEO_{2k}. Inset: SEM image of the produced Hex particles

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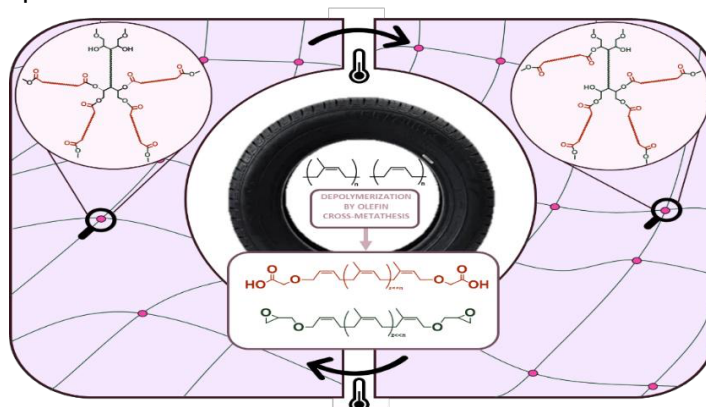
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PREPARATION OF ELASTOMERS FROM CHEMICALLY RECYCLED TIRE WASTE

E.Fondimare, I.Dez, and L.Le Pluart

Université Caen Normandie, ENSICAEN, Université Rouen Normandie, INSA Rouen Normandie, CNRS, Institut CARMen UMR 6064, 14050 CAEN, France
edgar.fondimare@ensciaen.fr

Valorization way of tire waste has a significant environmental impact due to the emission of toxic particles. Mostly composed of polydienes (such as polyisoprene and polybutadiene), these wastes offer a great potential for chemical upcycling to prepare elastomeric networks. In this context, olefin cross-metathesis reaction already proved to be a powerful tool for chemical recycling of tire waste.¹ It affords to simultaneously depolymerize polydienes into oligomers and end-chain functionalize the latters. This process requires an alkene with functional group used as chain transfer agent (CTA) and a Ru-based catalyst. Starting from a model high molar mass polyisoprene, our team successfully obtained in a controlled way, telechelic polymers with a molar weight varying between 3 kg/mol and 15 kg/mol and functionalized by various groups such as phosphonate, acetate and furyl.² Similarly, the epoxy/carboxylic acid pair was selected in the present study to enable the formation of reversible bonds through a thermally activated transesterification mechanism.³ From these functionalized polymers, covalent adaptative networks (CANs) named vitrimers can be prepared. Such innovative materials combine the mechanical and thermal properties of thermosets with the recyclability of thermoplastics. Our objective is to develop more sustainable vitrimers while promoting the valorization of tire waste. The results, including CTA synthesis, polyisoprene and tire waste depolymerization and the formulation of vitrimer materials, will be presented.



¹Yougourthen, B.; Chataigner, I.; Dez, I. Waste tire based thermoreversible elastomeric networks. *Eur. Polym. J.* **2025**, 227, 113770. DOI: 10.1016/j.eurpolymj.2025.113770.

²Perrot, A.; Renault, J.; Dez, I. Depolymerisation of polyisoprene by olefin cross-metathesis at equilibrium. *Polym. Degrad. Stab.* **2025**, 241, 111529. DOI: 10.1016/j.polymdegradstab.2025.111529

³Capelot, M.; Montarnal, D.; Tournilhac, F.; *et al.* Metal-catalyzed transesterification for healing and assembling of thermosets. *J. Am. Chem. Soc.* **2012**, 134 (18), 7664-7667. DOI: 10.1021/ja302894k

SWIFT AND EFFICIENT DIGITAL TESTS FOR "ON SITE" PFAS DETECTION

Micheline Draye¹, Guy Royal^{1,2}, Nathalie Cottin¹, Vincent Bouchiat³, Behnaz Djoharian³, Kokoura Mensah³

¹Univ. Savoie Mont Blanc EDYTEM, F-73000 Chambéry, France

²Univ. Grenoble-Alpes, DCM, F-38400 Grenoble, France

³GRAPHEAL, Biolabs Biopolis, 5 avenue du Grand Sablon 38700 La Tronche, France,
<https://grapheal.fr/>

micheline.draye@univ-smb.fr, guy.royal@univ-grenoble-alpes.fr, nathalie.cottin@univ-smb.fr,
vbouchiat@grapheal.fr, bdjoharian@grapheal.fr, kmensah@grapheal.fr

PFAS ("Forever Chemicals") represent a critical challenge in environmental monitoring due to their toxicity, persistence, and mobility¹. Current laboratory-based techniques (e.g., LC-MS/MS) offer high sensitivity but are costly, infrastructure-dependent, and unsuitable for rapid field deployment. Our joint Laboratory (FluoroGraph) aims addressing this gap by developing portable graphene-based electrochemical and field-effect transistor (FET) sensors for on-site PFAS detection and quantification. By coupling molecularly functionalized graphene layers with digital signal processing, the devices will achieve high sensitivity (ng·L⁻¹ range), rapid response times, and real-time data transmission. This innovation provides a scalable, low-power and low-cost solution for environmental pollution monitoring, regulatory compliance control, and risk assessment.

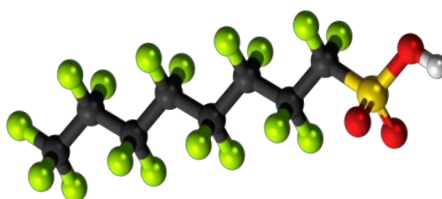


Figure 1: Chemical structure of an example of frequently investigated PFAS: perfluorooctanoic acid (PFOA).

¹ Draye, M.; Royal, G. Ultrasound-Driven Degradation of Organic Pollutants: Focus on Per- and Poly uoroalkyls (PFAS). *Encyclopedia of Green Chemistry*, Elsevier, 2025; pp. 483-491. DOI: 10.1016/b978-0-443-15742-4.00085-5

Synthesis of biaryl-atropisomers by central-to-axial chirality conversion

Léo Meyer,¹ Clément Lemaitre,² Adrien Quintard,³ John C. Stephens,⁴ Thierry Constantieux,² Xavier Bugaut^{1,2,5}

¹ Université de Strasbourg, Université de Haute-Alsace, CNRS, LIMA, UMR 7042, 67000 Strasbourg, France

² Aix Marseille Univ, CNRS, Centrale Marseille, iSm2, Marseille, France

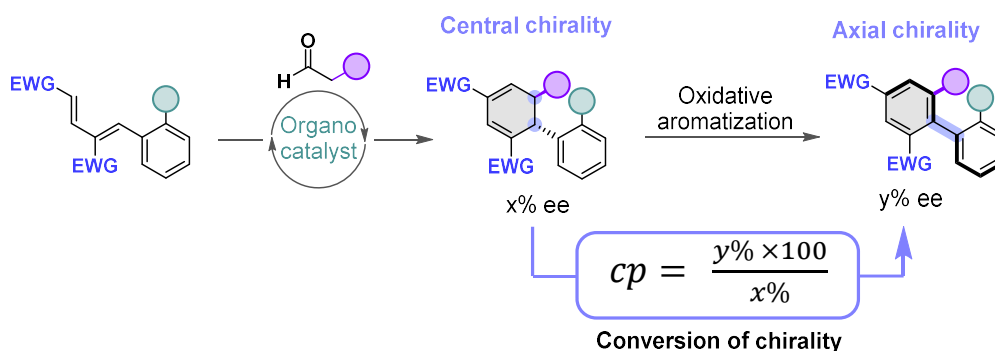
³ Université Grenoble Alpes, CNRS, DCM, 38000 Grenoble, France

⁴ Department of Chemistry, Maynooth University, Maynooth, Ireland

⁵ Institut Universitaire de France, 1 rue Descartes, 75231 Paris, France

leo.meyer5@etu.unistra.fr, xbugaut@unistra.fr

Atropisomers represent a unique class of axially chiral molecules whose chirality originates from a restricted rotation around a single bond, leading to the existence of stable rotamers.¹ Thanks to their structural features, atropisomers play a key role across diverse fields such as enantioselective catalysis, pharmaceuticals, natural products, or materials.¹ The growing interest for atropisomeric compounds highlights the necessity to develop new atroposelective synthetic strategies. Organocatalysis is particularly well suited for this purpose since it offers a broad range of enantioselective transformation under mild conditions, which is necessary to preserve the stereochemical integrity of these sensitive molecules.¹ In our approach, we combine the well-established control of central chirality offered by organocatalysis and the advantages of central-to-axial chirality conversion to access biaryl atropisomers stereoselectively.^{1,2,3} Specifically, our method involves the synthesis of enantioenriched aryl-substituted cyclohexadienes via the condensation of Michael acceptors (bearing two identical or distinct electron-withdrawing groups) with enolisable aldehydes. Subsequently, the controlled oxidative aromatization of the diene core affords atropoenriched molecules. Finally, these atropisomeric frameworks can be further diversified through post-functionalization, enabling the access to a wide variety of structures.



¹ Wang, Y.-B.; Tan, B. *Acc. Chem. Res.* **2018**, *51* (2), 534–547.

<https://doi.org/10.1021/acs.accounts.7b00602>.

² Lemaitre, C.; Perulli, S.; Quinero, O.; Bressy, C.; Rodriguez, J.; Constantieux, T.; García Mancheño, O.; Bugaut, X. *Molecules* **2023**, *28* (7), 3142. <https://doi.org/10.3390/molecules28073142>.

³ PhD thesis of Clément Lemaitre under the supervision of Xavier Bugaut and Thierry Constantieux, *Aix-Marseille Université*, **2021**, <https://theses.fr/2021AIXM0640>

VALORIZATION OF *CITRUS LIMETTA* PEEL FROM MOROCCO: EXTRACTION AND CHARACTERIZATION OF ESSENTIAL OILS

**Abderrahmane Faragi^{1,2} Khaoula Chattat^{1,3} Amal Sammama¹ Hinde Aassila²
Mohamed Najib Alfeddy¹**

1. Plant Protection Research Unit, Regional Center of Agricultural Research of Marrakech, National Institute of Agricultural Research, Avenue Ennasr, BP 415 Rabat Principal, 10090 Rabat, Morocco.

2. Faculty of Science & Technology, Agri-Food and Health Laboratory, Hassan First University of Settat, Settat 26000, Morocco.

3. Laboratory of Plant Biotechnology, Ecology and Ecosystem Valorization, URL - CNRST N°10, Faculty of Sciences, Chouaib Doukkali University, Av. Jabrane Khalil Jabrane, B.P. 299, 24000 El Jadida, Morocco.

Email address- faragi.doc@uhp.ac.ma

The valorization of by-products is a sustainable approach that reduces waste while generating value-added products. This study focuses on the recovery of *Citrus limetta* (sweet lime) peel from Morocco for the extraction of essential oils. The peels were subjected to hydrodistillation using a Clevenger-type apparatus. The extraction yield was determined, and the chemical composition of the essential oils was analyzed by gas chromatography–mass spectrometry (GC-MS).

In addition, the antioxidant activity was evaluated using DPPH and ABTS radical scavenging assays, while the antimicrobial potential was assessed against selected bacterial and fungal strains using the disc diffusion method.

Preliminary results revealed a high content of D-limonene, α -pinene, and γ -terpinene, associated with significant antioxidant capacity and notable antimicrobial effects. These findings highlight the potential of *Citrus limetta* essential oils as natural bioactive agents for cosmetic, pharmaceutical, and food applications, promoting sustainable valorization of Moroccan citrus by-products.

Keywords:

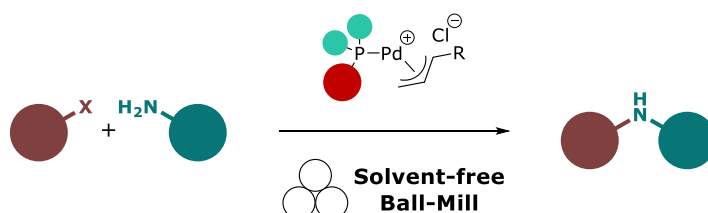
Citrus Limetta, Essential oils, Hydrodistillation, Antioxidant activity, Antimicrobial activity.

SOLVENT-FREE BUCHWALD-HARTWIG AMINATION: TOWARDS SUSTAINABLE CATALYSIS FOR SYNTHESIS

Deniz Karabiyikli,¹ Alexandre Saad,² Sokaina Hammoud,¹ Séverine Schneider,¹ Romuald Manca,² Jesus Raya,² Martine Schmitt,¹ and Frédéric Bihel^{1*}

¹Université de Strasbourg, Laboratoire d'Innovation Thérapeutique, CNRS/Unistra UMR7200, Strasbourg, France ; ²UMR7177 CNRS-Unistra, Laboratory of Membranes Biophysics and NMR, Institut de Chimie, Strasbourg, France
fbihel@unistra.fr

Amines are an integral part of biologically active molecules. The pharmaceutical industry heavily relies on robust and reproducible reactions for the formation of aryl amine moieties, with the Buchwald-Hartwig (BH) amination playing a central role. Its widespread use spans various stages of drug discovery and process development.¹ Traditionally, BH amination is performed in organic solvents such as THF and toluene. Unfortunately, at multi-kg scale pharmaceutical manufacturing, these conditions become extremely costly for the environment, with the solvents accounting for up to 80% of mass use.² To address this environmental concern and to provide efficient and safe methodology, our aim was to develop eco-compatible conditions for this crucial chemical transformation. We tackled this issue using mechanochemical ball milling.³ By eliminating the need for bulk solvent use, this strategy provides cleaner and ecological synthesis alternatives. While many cross-coupling reactions have been explored under mechanochemical conditions, research on solvent-free BH amination conditions in the literature remains limited.^{4–7} Building on our previous work developing a novel precatalytic system featuring [Pd(π -allyl)tBuXPhos]Cl in green alcoholic solvents,⁸ in this study, we demonstrate the application of the same precatalyst in mechanochemical solvent-free reaction conditions.⁹ We have demonstrated the coupling of aryl halides with various nitrogen-containing substrates including amines, amides, carbamates, ureas, among others. This expansion of reaction scope underscores the potential of our approach in facilitating sustainable and atom-efficient synthesis for synthesis of biologically active molecules.



[1] J. Magano, J.R. Dunetz. *Chem. Rev.* (2011) 111, 2177–2250 ; [2] S. Kar *et al.* *Chem. Rev.* (2022) 122, 3637–3710; [3] J.-L. Do, T. Friščić. *ACS Cent. Sci.* (2017) 3, 13–19 ; [4] Q.-L. Shao, Z.-J. Jiang, W.-K. Su, *Tetrahedron Lett.* (2018) 59, 2277–2280; [5] K. Kubota *et al.* *Nat. Commun.* (2019) 10, 111 ; [6] K. Kubota *et al.* *ACS Sustain. Chem. Eng.* (2020) 8, 16577–16582; [7] Q. Cao *et al.* *Org. Biomol. Chem.* (2019) 17, 1722–1726 ; [8] P. Steinsoultz *et al.* *ACS Catal.* (2022) 12, 560–567 ; [9] Karabiyikli *et al.* *ChemSusChem* (2025) 18, 13, e202500545.

MACROMOLECULAR CROWDING AS A NEW STRATEGY TO MODULATE NUCLEATION AND CRYSTALLIZATION OF ZEOLITE

Samouh Sarah¹, Nuss Amélia¹, Lutzweiler Gaëtan¹

¹Institute for Chemistry and Processes for Energy, Environment and Health (ICPEES UMR 7515)), University of Strasbourg, France

Green Chemistry guides the development of more efficient and less polluting processes. In this context, zeolites are essential materials. These crystalline and microporous aluminosilicates exhibit well-defined porosity and high stability, appearing as benchmark materials for green applications such as heterogeneous catalysis and adsorption.

Their synthesis generally involves a hydrothermal treatment of a preformed gels containing silicates and aluminates species, with sometimes an organic template. Interestingly, organic additives can influence this process by acting on nucleation and crystal growth. In this context, polyethylene glycol (PEG 20 000) was introduced as an organic additive to investigate the effect of macromolecular crowding on zeolite formation.

Macromolecular crowding is well known in biological systems. It relies on the exclusion of free volume by large macromolecules, which can be mimicked by polymer chains in vitro. This can induce phase separation, where droplets are formed typically enriched in a given type of molecules, surrounded by a more dilute medium. In the droplets, a restricted diffusion can be observed, as well as modified rates of biochemical reactions. PEG 20 000 due to its high solubility and molecular weight can reach concentrations where polymer chains overlap, thus forming confined spaces, potentially impacting crystallization of zeolites and crystal morphology.

Zeolites were hydrothermally synthesized, PEG was added at different concentrations and the materials were characterized by x-ray diffraction and SEM. As shown in Figure 1, PEG induces a liquid-liquid phase separation, creating heterogeneous environments for crystallization.

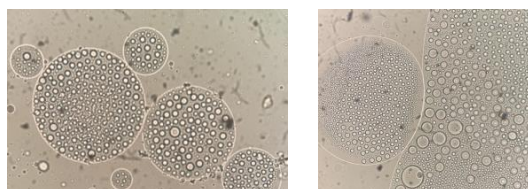


Figure 1. Phase separation observed under optical microscopy after PEG addition

SEM images (Figure 2) reveal that before calcination, crystals are dense and disordered, while after calcination at 500°C, porous and rough structures appear. This demonstrates that PEG acts as a templating and structuring agent, promoting hierarchical porosity.

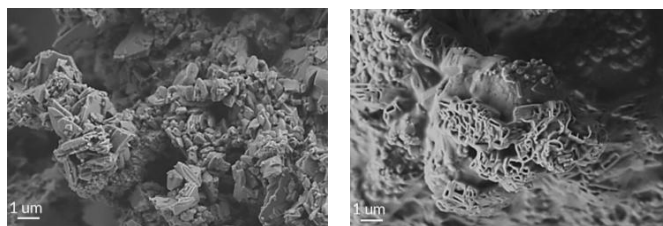


Figure 2. SEM images before and after calcination of zeolite synthesized with PEG 20 000

In conclusion, PEG modifies the morphology, crystallinity and porosity of zeolites through macromolecular crowding effects.