Réseau des Jeunes Chimistes
Société Chimique de France

École Doctorale
Sciences Chimiques Balard

BOOK OF ABSTRACTS

2023 - 11e EDITION

JMJC

JOURNÉES MEDITERRANÉENNES DES JEUNES CHERCHEURS

9th & 10th November 2023 - Institut Botanique, Montpellier

NJC ROYAL SOCIETY OF CHEMISTRY

VWR Part of Avantor

CEM

IBMM Institut des Biomolécules Max Mousseron

ICGM Institut Charles Gerhardt Montpellier

ICSM

iem Institut Européen des Membranes

MAISON de la CHIMIE
l'Adresse de votre événement

POLE chimie Balard

SCF

Ecole Doctorale
Sciences chimiques / ED 250

UNIVERSITÉ DE MONTPELLIER

Word from the organizing comitte

Every 2 years, the Young Chemists' Network of the Société Chimique de France from Occitanie Méditerranée (RJ-SCF-OM) and Provence Alpes Côte d'Azur (RJ-SCF-PACA) join their efforts with the Doctoral School « Ecole Doctorale Sciences Chimiques BALARD » (ED SCB, 459) to organise the Journées Méditerranéennes des Jeunes Chercheur(e)s (JMJC) in Montpellier.

The 11th edition of this general conference targeting students, doctoral students and young researchers in particular will take place on the 9th and 10th November 2023, with the aim of bringing together those involved in chemistry in the south of France (from Montpellier to Nice). These days will give them the opportunity to present their work and meet internationally renowned speakers. To this end, the conference will be organized into several sessions, including plenary lectures and oral and written communications (posters). The congress is organized around 3 topics (biomolecules, material chemistry and biochemistry) to match with the richness and the plurality of the research institutes in Montpellier. These different sessions will encourage exchanges between the various players in the field of chemistry from the academic and industrial sectors.

We hope that this 2023 edition will be as successful as the previous editions!

The organizing committee of the JMJC 2023.

Organizing comitte

Young Chemists' Network of the Société Chimique de France (RJ-SCF)

- ***Occitanie Méditerranée Section (RJ-SCF-OM)***

Director : Jean Felix BOUE
Secretary : Florian LUTTRINGER
Treasurer : Raphaël EL BEKRI SAUDAIN

Active members : Adelaïde GARTILI, Lilian GENILLER, Jordan LEHOUX, Karen MENGUE NDONG, Maiko MONTEIL, Ludivine POYAC, Anu VASHISHTHA.

- ***Provence Alpes Côte d'Azur Section (RJ-SCF-PACA) :***

Jessica RODRIGUES

Doctorale School Sciences Chimiques Balard (ED SCB)

Bureau

Director : Marc CRETIN
Deputy Director: Claire LONGUET
Administrator : Charlène ERIMIAN

Presentation of the event

The 2023 edition of the JMJC will take place on the 9th and 10th November 2023 in Montpellier. These two full days will provide an opportunity for chemistry actors from the south of France to meet in the same place to share and discover their respective work.

Held alternatively in the PACA region (Marseille, Toulon, Nice) and the OM region (Montpellier), the JMJCs are mainly aimed at a young audience of students, doctoral students and post-doctoral fellows. This major event gives chemists from these two major regions of southern France the opportunity to meet, exchange ideas and debate over two days, through conferences and informal get-togethers in a friendly atmosphere.

Doctoral students and young researchers will have the opportunity to present their work in the form of oral or written papers (posters) during three themed half-days covering all areas of chemistry. Internationally renowned speakers will be invited to discuss their work with experienced researchers. Finally, industrial partners will be invited to represent all the different players and sectors in chemistry and to encourage links between industry and academia.

Acknowledgments

We would like to thank all the people who helped us directly or indirectly both in the organization before and during the congress. Nothing would have been possible without you!

First, we would like to begin to express our thanks to the "BALARD Chemical Sciences" doctoral school (ED 459) and in particular its director, Mr. Marc CRETIN, who have unreservedly accepted to participate in the organization of this event. This support is essential to the holding of the JMJC! We would also like to thank our young chemist counterparts from the PACA regional section of the French Chemical Society (RJ-SCF-PACA), with whom we alternate the organization of this congress.

We would like to extend our sincere thanks to our guest speakers, Prof. Claude GRISON, Dr. Gaëlle CHOURAQUI, Prof. Kenji NAGATA and Dr. Diego Moreno Martínez, who have come to Montpellier to honor us with their presence. We are truly delighted and lucky to welcome you to Montpellier and are convinced that the presentation of your work will be very enriching for young chemists. We hope you will have a pleasant stay with us!

Thanks should also go to all our partners:

- The 4 Montpellier chemistry research institutes and in particular their directors for the financial support, Mr. Pascal DUMY for **IBMM**, Mr. Eric CLOT for **ICGM**, Mr. David CORNU for **IEM** and Mr. Stéphane PELLET-ROSTAING for **ICSM**.
- The **Pôle Chimie**, in particular Ms. Pauline CHARRIAUX, Ms. Héléa KHAIZOURANE and Mr. Philippe MIELE, Director of the Pôle Chimie MUSE.
- The New Journal of Chemistry to have contributed generously to the funding of the communications awards. This enables young chemists to be encouraged in their research and to attend further conferences.
- The **Occitanie-Méditerranée regional section of the French Chemical Society** (SCF-OM), and in particular its president Ms Armelle OUALI for her advices and availability and Yaovi HOLADE for his work.
- The Montpellier University for allowing us to hold this conference at the Botanical Institute.
- The Fondation de la Maison de la Chimie, in particular Ms. Sophie TATIN and Mr. Henri DUGERT, its General Secretary.
- The "**Sea and Science" doctoral school** of Toulon (ED 548) and "**Chemical Sciences" doctoral school** of Aix-Marseille (ED 250).
- The sponsors of this conference for the financial support that makes this conference possible to be held year after year: **VWR**, **CEM**

Finally, thank you all – audience and speakers – for being present for this eleventh edition of the Mediterranean Young Researchers Days which we hope you will enjoy!

Thank you everyone!

The young chemists' network of the Occitanie-Méditerranée section of the French Chemical Society.

Program

Thursday 09th November		
09h00 - 09h30		*Registration & Opening*
09h30 - 10h30		**Prof. Claude GRISON** ***Montpellier University*** **"insérer Titre présentation"**
10h30 - 11h00		*Coffee break*
11h00 - 11h20	**F. ABDEL SATER** ICGM	"Magneto-luminescent iron oxide nanoplatform: towards temperature control in photothermia and magnetothermia"
11h20 - 11h40	**M. HAUSDORFF** IBMM	"Adenosine mimetics as selective and potent inhibitors of coronavirus nsp14 N7-methyltransferases"
11h40 - 12h00	**S. ATHAR** ICGM	"Data-driven discovery of efficient thermoelectric materials using symbolic regression"
12h00 - 12h05		**Partner presentation : CEM**
12h05 - 13h30		*Lunch Break & Poster session*
13h30 - 14h30		**Dr. Gaëlle CHOURAQUI** ***Aix-Marseille University*** "Designing donor-acceptor cyclopropanes for the synthesis of valuable building blocks"
14h30 - 14h50	**S. CHAISE** IBMM	"The ring rules the shape: a γ-peptide story"
14h50 - 15h10	**S. LAVIEVILLE** ICGM	"Trifluoromethylated N,O- and N,S-acetals: new reversible functions for vitrimer application"
15h10 - 15h30	**V. NAVARRO** IBMM	"Ball-milling strategies for the synthesis of dinucleotides and analogues"
15h30 - 16h00		*Coffee break*
16h00 - 16h20	**M. MONTEIL** ICGM	"Development of a personalized 3D printed form loaded with MCM-41 Silica"
16h20 - 16h40	**A. GACOGNE** IBMM/ICGM	"Towards γ-Foldamers as bifunctional enamine/iminium organocatalysts in enantioselective transformations"
16h40 - 17h00	**M. ABDELFADEEL** ICGM	"High performance cryogels based on Carboxymethylcellulose and loaded with reduced graphene oxide and nickel oxide for supercapacitors applications"
18h00		***Dinner Cocktail (Salle Pétrarque)***

Friday 10th November		
09h00 - 09h10		*Welcome speech*
09h10 - 09h30	**S. JAYAKUMAR** IEM	"Hydrophobic ceramic capillary membranes applied for desalination by membrane distillation"
09h30 - 09h50	**J. TANEPAU** IBMM/ICGM	"Mechanochemical ATRP: Practical conditions for liquid and solid monomers controlled polymerization in the ball mill"
09h50 - 10h10	**H. CARVAILLO** IBMM	"Design and synthesis of Kallikrein 6 inhibitors for Multiple Sclerosis treatment"
10h10 - 10h30	**E. MUMBA MPANGA** ICGM	"Solid-state chemistry shuffling of alkali ions towards new layered oxide materials"
10h30 - 11h00		*Coffee break*
11h00 - 11h20	**Dr. D. MORENO** CEA-Marcoule	**Winner of the SCF-OM 2022 Thesis Prize**
11h20 - 11h40	**W. NZODOM** ICSM	"Synthesis of zeolite A under sonohydrothermal conditions and investigation of its conversion into sodalite"
11h40 - 12h00	**M. LAVAYSSIERE** IBMM	"Amidation by reactive extrusion for the synthesis of active pharmaceutical ingredients teriflunomide and moclobemide"
12h00 - 12h05		**Partner presentation : CEM**
12h05 - 13h30		*Lunch Break & Poster session*
13h30 - 13h50	**I. STROIA** IEM	"Tuning transmembrane transport by playing with C-H donor strength in a series of bis(cyanostilbene) podants"
13h50 - 14h10	**I.-M. ANDREI** IEM	"Selective water pore recognition and transport through self-assembled Alkyl-Ureido-Trianglamine artificial water channels"
14h10 - 14h30	**P. GUERIN** iSm2	"Chiral biaryls: from axial to planar chirality using Kumada-Tamao-Corriu coupling"
14h30 - 14h50	**F. AZROUR** ICGM	"Structural study of piezoelectric LnCa4O(BO3)3 at high pressures and cryogenic temperatures"
14h50 - 15h20		*Coffee break*
15h20 - 16h20		**Pr. Kenji NAGATA** ***Nagoya Institute of Technology*** "Electrical conductivity and phase morphology of graphene-filled Polyethylene/Polypropylene composites"
16h20 - 17h00		***Prizes & Closing***

Abstracts

- **4 guests speakers**

Dr. Gaëlle CHOURAQUI

Institute of Molecular Sciences of Marseille (iSm2)

Aix-Marseille University

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Pr. Claude GRISON

Laboratory of Bio-inspired Chemistry and Ecological (ChimEco)

Montpellier University

p.10

Pr. Kenji NAGATA

Nagoya Institute of Technology

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Dr. Diego Moreno Martínez

CEA Marcoule

Montpellier University

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DESIGNING DONOR-ACCEPTOR CYCLOPROPANES FOR THE SYNTHESIS OF VALUABLE BUILDING BLOCKS

Gaëlle CHOURAQUI,[a] Paola NAVA,[a] Laurent COMMEIRAS,[a] Jean-Luc PARRAIN,[a] Kévin MASSON,[a] Bohdan BILETSKYI,[a] Maxime DOUSSET,[a] Pierre COLONNA,[a] Michel GIORGI,[b] Jean-Valère NAUBRON,[b] Sara CHENTOUF [b]

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Keywords: Benzocyclobutene, Donor-acceptor Cyclopropane, 8-membered ring, Rearrangement.

Donor-Acceptor Cyclopropanes (DACs) are remarkable chemical species that have been extensively used as valuable 1,3-dipole synthetic building blocks.[1] The opposing electronic properties of the vicinal substituents combined with the ring strain of the cyclopropane (~ 27.5 kcal.mol^{-1}) not only direct but also facilitate the bond scission. This *push-pull* effect has found wide applications in natural product synthesis and drug development. Lately, authors have been interested in studying different donor patterns and step away from the classical O, N or phenyl donor substituents. Interestingly, two different groups showed that the cyclopropyl group can act as an excellent donor one (Fig 1, eq. 1).[2] The authors demonstrated that various (3+n) cycloaddition reactions could be accomplished, and the corresponding cyclic systems obtained were substituted with the valuable small ring. Inspired by this work, our group also contributed to the field.
Herein, we report that a common unusual vinylogous DAC **1** could lead, depending on the conditions used, either to the challenging carbocyclic eight-membered ring **2** (Fig. 1, eq. 2)[3] or the interesting benzocyclobutene building block **3** (Fig. 1, eq. 3).

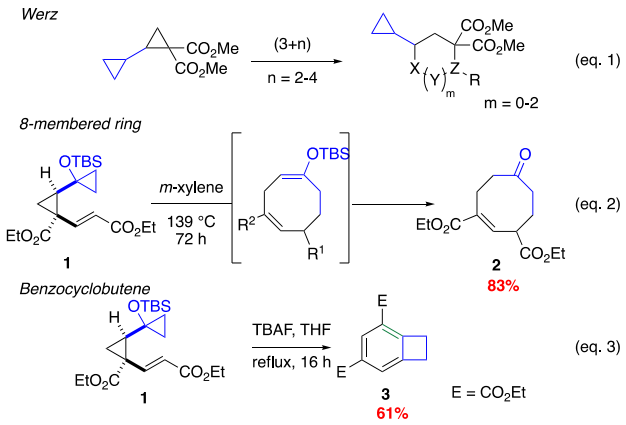

Fig. 1 The cyclopropyle as a donor group.

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“WHAT IS CHEMISTRY FOR ECOLOGY”

Prof. Claude GRISON

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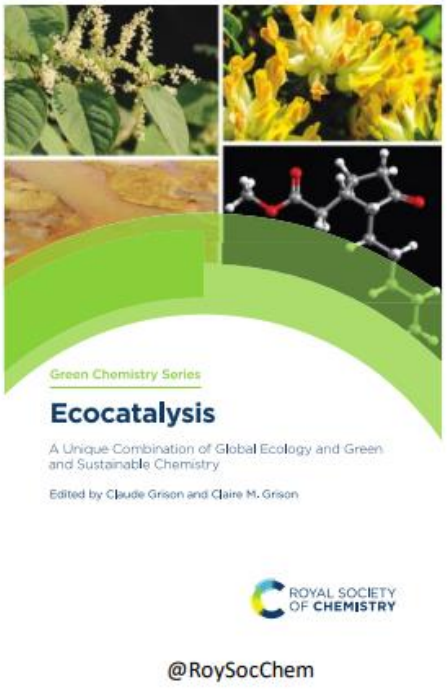
Facing global crises of many sorts, chemistry must integrate the social and economic dimensions of these processes, but also eco-responsibility. In this context, the laboratory of Bio-inspired Chemistry and Ecological Innovations is developing a new green sector, which is based on a breakthrough innovation in chemistry, called ecocatalysis or ecological catalysis. Its originality is based on an unusual concept: combining Nature, Ecology, Chemistry, Research and Industry. However, such associations are far from being evident. The objective of this research is to demonstrate that it is possible to integrate economic activity, technological optimism and the search for innovative environmental strategies as a real vector of sustainable development.



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3. http://www.chimeco-lab.com

“ELECTRICAL CONDUCTIVITY AND PHASE MORPHOLOGY OF GRAPHENE-FILLED POLYETHYLENE/POLYPROPYLENE COMPOSITES”

Prof. Kenji Nagata

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Conductive composites of polypropylene (PP) and polyethylene (PE) filled with thermally reduced graphene oxide (TRG) were prepared using two different processing sequences. One was a one-step processing method in which the TRG was simultaneously melt blended with PE and PP, called TRG/PP/PE. The second was a two-step processing method in which the TRG and the PP were mixed first, and then the (TRG/PP) masterbatch was blended with PE, called (TRG/PP)/PE. The phase morphology and localization of the TRG in TRG/PP/PE and (TRG/PP)/PE composites with different PP/PE compositions were observed by transmission electron microscopy (TEM) and scanning electron microscopy (SEM). The TRG was found to be selectively dispersed in the PE phase of the TRG/PP/PE composites, resulting in a low percolation threshold near 2.0 wt%. In the (TRG/PP)/PE composites, the TRG was selectively located at the PP/PE blend interface, resulting in a percolation threshold that was lower than 1.0 wt%. With the addition of 2.0 wt% TRG, the (TRG/PP)/PE composites exhibited a wide range of electrical conductivities at PP/PE weight ratios of 10 w/90 w to 80 w/20 w.

In addition to “Graphene-filled Polyethylene/Polypropylene Composites”, we would be grateful if we could introduce you to our research on thermally conductive polymer blends.

MOLECULAR DYNAMICS STUDY OF THE URANIUM(VI) SEPARATION USING SOLID SUPPORT

Diego Moreno Martinez, Dominique Guillaumont and Philippe Guilbaud

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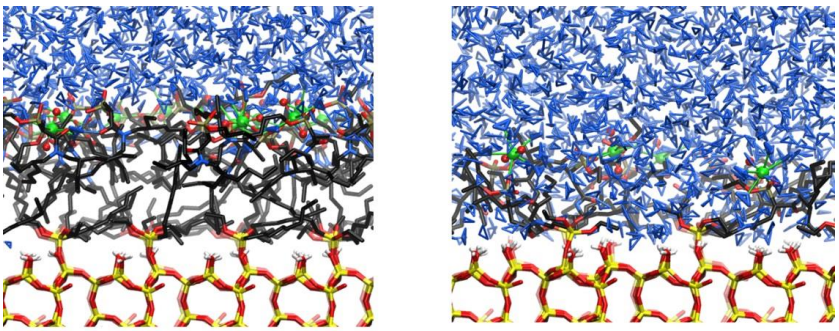
The uranium extraction plays an essential role in the nuclear fuel cycle. The supported liquid extraction, using functionalized mesoporous silica, represents a promising alternative to the liquid/liquid extraction processes.[1] In fact, the compactness of these solid supports, and the facility of implementation associated to the reduction of organic effluents, give to this system great competitive advantages. Despite previous experimental studies about these solid/liquid systems, a detailed characterization at the molecular and supramolecular scale is missing, and the uranium extraction mechanisms are not understood. The objective of this research, centered on theoretical chemistry studies (especially by molecular dynamics), is to rationalize the behaviors that have been experimentally observed and to provide comprehension elements by simulating the solid/liquid media. These studies presented technical, conceptual and fundamental challenges: a) The parametrization of a model, for the uranium(VI) molecular cation, with a simplified consideration of polarization effects in order to perform long simulations, while describing correctly the speciation,[2] b) The conception of representative model of solid supports, and c) The production of long simulation times allowing to observe the uranium extraction mechanisms. The analysis of the simulations reveal that the supramolecular organization of the solid/liquid interface is particularly different depending on the incorporation mode of extractant molecules in the solid support (see Fig. 1). Moreover, the uranium species formed in the solid/liquid interface are stabilized not only by complexation of extractants but also by weak interactions network. The results can explain experimental observations and show how coupling molecular modelling with experiments leads to a fine exploration of the molecular interactions and supramolecular organization of such systems.



Impregnated extractants *Grafted extractants*

Figure: Molecular dynamics snapshots of the solid/liquid interface supramolecular organization depending on the incorporation mode of extractant uranium molecules.

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Abstracts

○ 20 oral communications

Magneto-luminescent iron oxide nanoplatform: towards temperature control in photothermia and magnetothermia

Farah Abdel Sater[a], Gautier Felix[a], Saad Sene[a], Joulia Larionova[a] and Yannick Guari[a]

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Iron oxide nanoparticles, thanks to their superparamagnetic and optical properties, have the potential to generate heat. This characteristic offers promising applications in hyperthermia treatment, catalysis, and radical release[1]. A better understanding and control of the temperature elevation on the surface of the NPs represents a challenge. In this study, we are expanding our investigation into the development of multifunctional nanoplatforms consisting of an iron oxide@silica with mesoporous silica shell into which luminescent lanthanide-based complexes are grafted to serve as nanothermometers[2,3]. The resulting material is expected to perform magnetothermia and/or photothermia and simultaneously measure the local temperature rise.

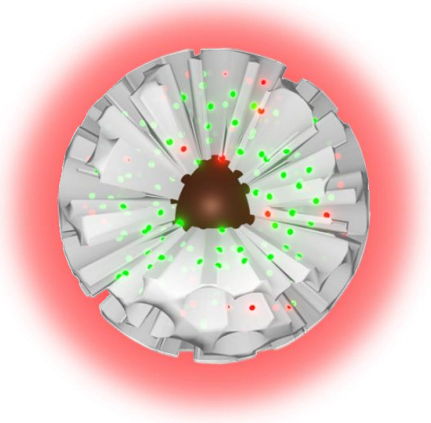

Figure 1: Iron oxide@silica[Ln-complex] nanoplatrform.

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Adenosine mimetics as selective and potent inhibitors of coronavirus nsp14 N7-methyltransferases

Marcel Hausdorff[a], Adrien Delpal[b], Sarah Barelier[b], Laura Nicollet[a], Bruno Canard[b], Franck Touret[c], Agathe Colmant[c], Bruno Coutard[c], Jean-Jacques Vasseur[a], Etienne Decroly[b], and Françoise Debart [a]

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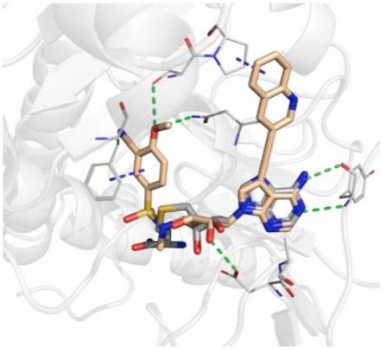
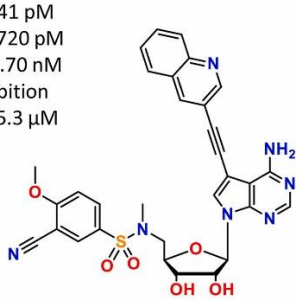
Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) is the third highly pathogenic coronavirus (after SARS-CoV and MERS-CoV), that emerged in 2019. Currently, treatments for diseases caused by CoVs are still limited and none have been found to directly counteract the viral replication pathway. Therefore, there is a need to identify effective treatments to cure COVID. Enzymes involved in SARS-CoV-2 RNA capping are essential for viral RNA stability, mRNAs translation, and virus evasion from innate immunity, making them attractive targets for antiviral agents[1].

In 2020, our group pioneered the development of selective SARS-CoV *N*7-guanine methyltransferase (MTase) inhibitors designed as adenine dinucleosides mimicking *S*-adenosyl-L-methionine (methyl donor in the *N*7-methylation of the cap) analogues[2]. Next, we optimized the design of the initial inhibitors and we synthesized a new library of adenosine-derived inhibitors. Seven compounds showed noteworthy nanomolar inhibition against SARS-CoV-2 *N*7-MTase nsp14[3]. In the present work, the adenine nucleobase was replaced by hypoxanthine, *N*6-methyladenine, or *C*7-substituted 7-deaza-adenine and a C7-quinoline 7-deaza-adenosine analogue showed a subnanomolar IC_{50} against CoVs nsp14. These new inhibitors displayed high selectivity against other MTases (viral or human), resulting probably from the positioning of the quinoline in a SAM entry tunnel present in the nsp14 structure and absent in other MTases[4].



IC_{50} (SARS-CoV nsp14) = 141 pM
IC_{50} (SARS-CoV-2 nsp14) = 720 pM
IC_{50} (MERS-CoV nsp14) = 2.70 nM
IC_{50} (DV3 ns5) = no inhibition
IC_{50} (human RNMT) = 165.3 µM



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Data-driven discovery of efficient thermoelectric materials using symbolic regression

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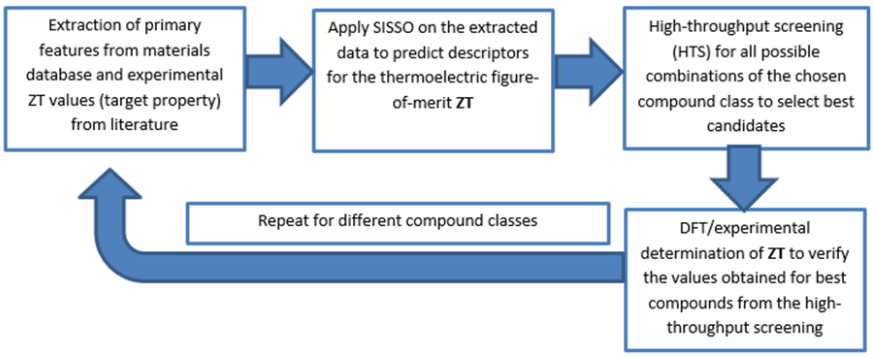
The demand for sustainable energy has sparked huge interest in finding novel and efficient energy conversion materials. Thermoelectric (TE) materials which can produce electricity, both directly and reversibly, from waste heat have particularly garnered significant attention given the fact that almost 60% of the fossil fuel energy is lost mostly as heat[1,2]. While machine learning can facilitate the accelerated discovery of efficient thermoelectric materials from the enormous configurational space of different compounds, the scarcity of experimental TE datasets limits the application of several conventional ML techniques. Moreover, their "black-box" nature fails to give structure-property relationship insights to develop criteria for high performing materials. Herein, we propose using a novel symbolic regression-based ML technique, SISSO (Sure Independent Screening – Sparsifying Operator) to determine physically interpretable descriptors for predicting the TE figure-of-merit, ZT, from a relatively small dataset of TE materials[5]. Using SISSO for a promising class of TE materials as an example, we demonstrate how from a relatively small set of training data as well as atomic features a complex target property like ZT can be predicted by obtaining mathematically explicit descriptors.



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The ring rules the shape: a γ-peptide story.

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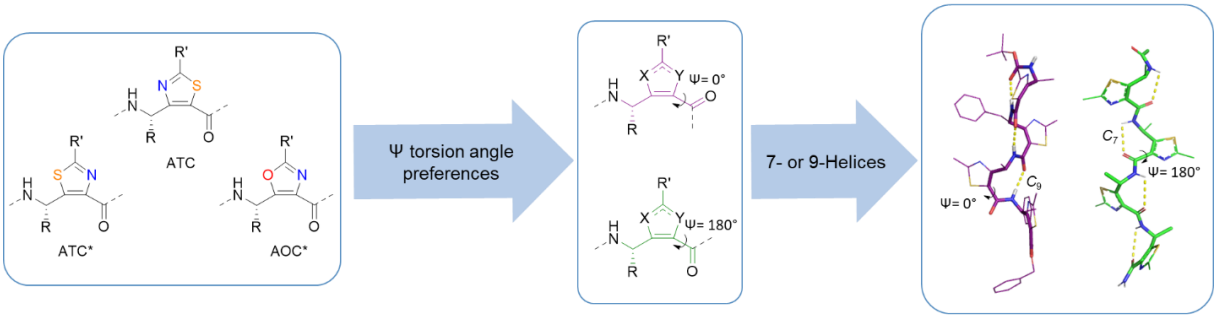
Heterocycles are widely used in many areas of organic chemistry to develop therapeutics and peptidomimetics.[1] They can orient molecular conformation in different ways since heteroatoms are hydrogen bond donors and acceptors, have negative and positive partial charges, and thus are key players in a wide range of interactions.[2] The last decade, we developed γ-peptide foldamers incorporating highly constrained five-membered heterocyclic γ-amino acids built around a thiazole, named ATC for 4-Amino(methyl)-1,3-Thiazole-5-Carboxylic acid.[3] We showed that ATC induces original 9-helix[4] and 9/12-ribbon[5] in γ- and α/γ-peptides, respectively.
In this study, according to conformational searches, we hypothesized that varying the nature of the heterocycles in γ-peptide backbones may offer new prospects to tune the stability of existing helices and theoretically allows to reach new architectures. We first developed robust synthesis pathways to access to enantiomerically pure thiazole- and oxazole-based analogs of ATC so called ATC* (5-amino(methyl)-1,3-thiazole-4-carboxylic acids) and AOC* (4-amino(methyl)-1,3-oxazole-5-carboxylic acids). We extensively studied the conformational preference of the corresponding oligomers by DFT, FTIR, XRD, CD, and NMR in a wide range of solvent conditions. We obtained a 7-Helix structure never described before whose stability varies with the chain-length. Interestingly, we observed a solvent-dependent conformational switch between the 7- and the 9-Helices.



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Trifluoromethylated N,O- and N,S-acetals: new reversible functions for vitrimer application

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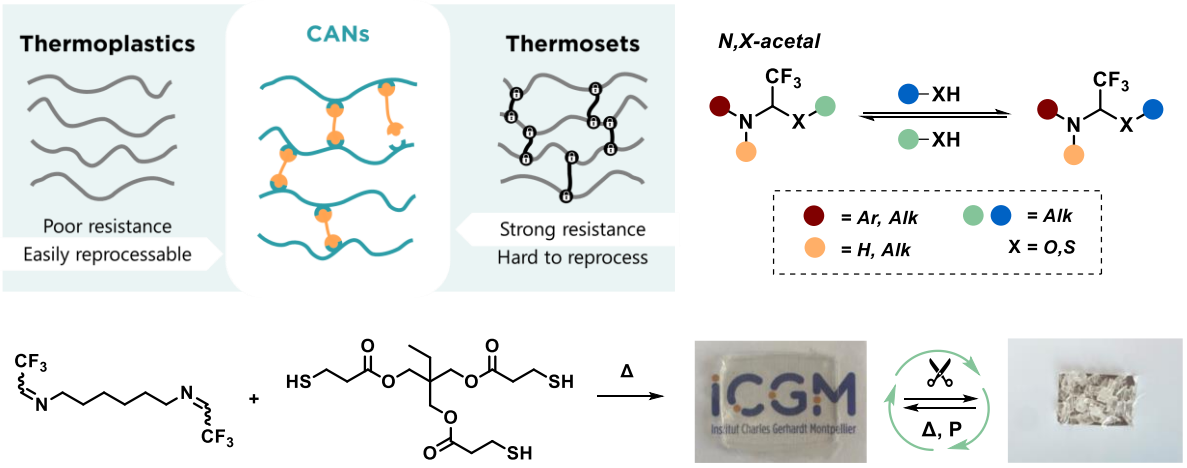
Vitrimers (or CANs), introduced by L. Leibler in 2011, are a new class of polymers combining the reshaping and recyclability properties of thermoplastics with the mechanical and chemical properties inherent to thermosets.[1-3] Vitrimers have a 3D crosslinked structure similar to thermosets, but feature exchangeable/reversible crosslinking bonds. The incorporation of fluorinated groups is a means to activate functional groups in order to promote exchange reactions without the need of a catalyst[4-8], but also to access new functional groups which are usually too unstable, such as N,O-acetals and N,S-acetals. These fluorinated acetals can undergo respectively alcohol and thiol exchanges. This work presents the synthesis of trifluoromethylated monomers and their incorporation into new N,O-acetals and N,S-acetals vitrimers.



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Ball-milling strategies for the synthesis for the synthesis of dinucleotides and analogues

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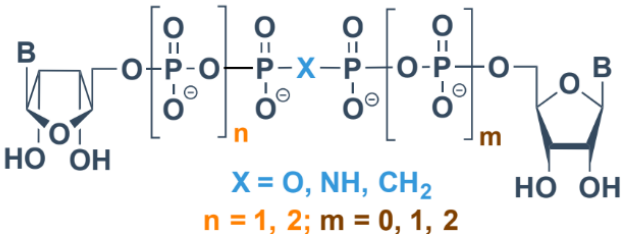
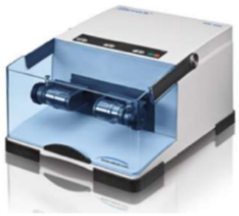
Dinucleoside 5',5'-polyphosphates (NpnNs) are endogenous substances that play important intra- and extracellular roles in various biological processes, such as cell proliferation, regulation of enzymes, neurotransmission, platelet disaggregation and modulation of vascular tone.[1] These compounds and their analogues are highly relevant in the medical field, as illustrated by Up4U, a P2Y2 receptor agonist used as a drug for treating dry eye syndrome.[2] Due to their importance in biological processes and their potential as therapeutic agents, several methods have been developed to access to these compounds and their structural analogues.[3] Most of them present important drawbacks, such as the use of non-volatile and harmful solvents (mostly DMF), preparation of substrates or phosphorus reagents in their trialkylammonium form due to solubility issues, anhydrous conditions, and fastidious purifications. Thus, we have developed one-pot, protecting-group free approaches, which are user-friendly and reliable, for the preparation of dinucleotides starting from nucleoside 5'-monophosphates or inorganic polyphosphates using N,N'-carbonyldiimidazole as activating agent.[4] Benefits of these one-pot methods include convenient set-up, short reaction time, and good to high conversion rates. and. These solvent-assisted mechanochemical approaches allowed to prepare dinucleoside 5,5'-polyphosphates, as well as analogs.





Altogether, our studies offer new perspectives for the development of greener approaches to access a wide range of nucleotide derivatives and analogs.

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Development of a personalized 3D printed form loaded with MCM-41 silica

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Chronic diseases require frequent administration per day leading to non-observance of the treatment. Furthermore, these treatments may concern patients (such as newborn or children) or active pharmaceutical ingredients (API) with a narrow therapeutic window needing personalized treatment with adapted dose (per kg weight). In these specific cases, personalized extended-release forms need to be developed to reduce the frequency of administration and adapt API dose.

Among innovation research on extended release form, ordered mesoporous silica (MCM-41) is a particularly appealing material due to its high pore volume, enabling high drug loading. It also features an organized pore network with a narrow pore size distribution, which can be adjusted to control drug release. Commercial silica are available but direct loading method allows simultaneous the mesostructuration of the silica and drug incorporation, which is time-saving[1,2]. Concerning the development of personalized form, pharmaceutical 3D printing has emerged as a potential solution. Among the various 3D printing techniques, Fused Deposition Modeling (FDM) stands out due to its low cost and accessibility as evidenced by the increasing number of research articles published in the last decade (4-fold between 2012 and 2022)[3].

Thus, our work aims to develop a personalized FDM 3D printed form loaded with MCM-41 silica to control drug release in order to improve treatment compliance and safety. MCM-41 silica was synthesized and loaded in a one-pot step using Poly(poly(ethylene glycol)-methyl ether acrylate)-b poly(sodium 4-vinylbenzenesulfonate) (PEO-PSS) copolymer in the presence of silica precursors (TEOS) and neomycin as a model drug. The resulting MCM-41 was characterized using BET, TEM, and the drug load was quantified. Subsequently, PEG filaments loaded with MCM-41 silica were prepared using hot melt extrusion and printed using FDM[1]. A drug release study was then conducted on the loaded hybrid materials and material formulation will be adapted to obtain required form.

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Towards γ-Foldamers as Bifunctional Enamine/Iminium Organocatalysts in Enantioselective Transformations

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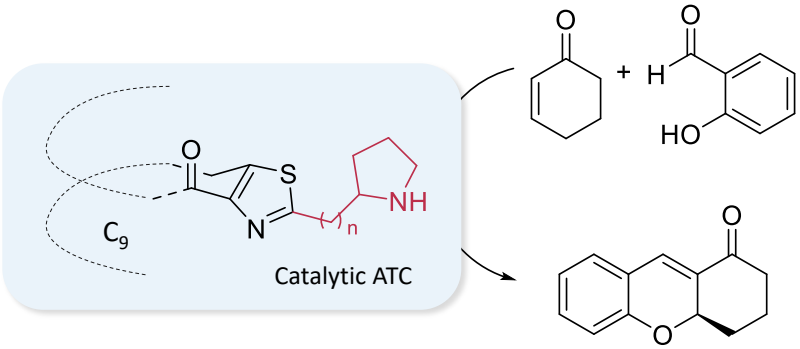
In the field of ecofriendly chemical transformations, considerable attention has been paid to organocatalytic processes to achieve carbon-carbon bond forming reactions. In such a context, great achievements have been reached following a bioinspired approach in constructing catalytic sites from short artificial folded oligomers (so call foldamers).[1] Over the last years, our group have explored a class of heterocyclic γ-peptides built around a thiazole ring, named ATCs (4-amino(methyl)-1,3-thiazole-5-carboxylic acids), adopting a highly stable helix structure.[2] Recently, these γ-peptides have been validated as synthetically tractable platforms for a nitro-Michael addition reaction.[4] In a natural extension of the undertaken studies, we now intend to consider ATC foldamers in the context of a more challenging reaction, consisting in the oxa-Michael aldol addition reaction between salicylaldehyde and cyclohexanone. We herein report the design and synthesis of the catalytic ATC and the optimization of the reaction conditions. The insertion of the catalytic monomer in ATC-based γ-peptide foldamers offers the opportunity to perform dual activation of both reacting partners, with the aim to increase both the turn-over and the chiral induction of the transformation.[5]



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High performance cryogels based on Carboxymethylcellulose and loaded with reduced graphene oxide and nickel oxide for supercapacitors applications

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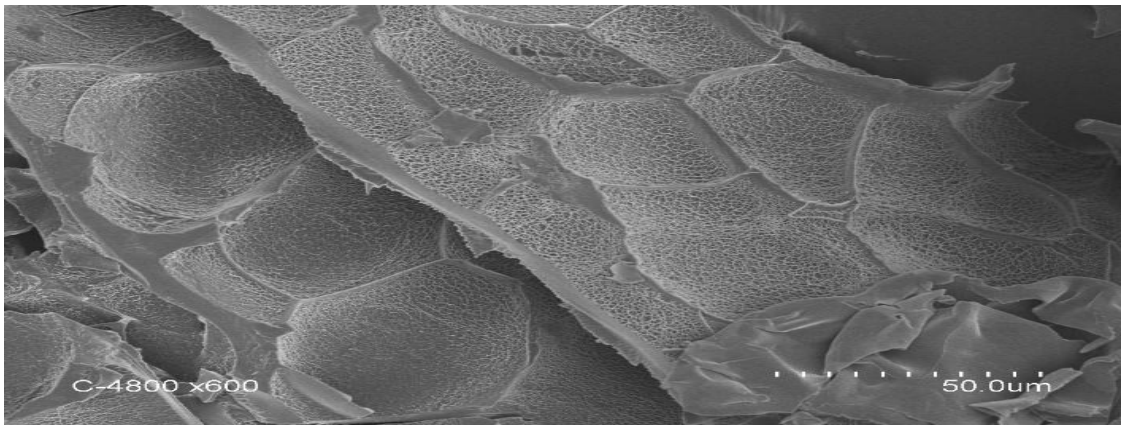
Regarding the high challenges for better energy storage units and supercapacitors for applications in electrical devices, great researches have been done to satisfy this high demand. In this work, we are focusing on designing new electrically conductive cryogels based on carboxymethyl cellulose-g-poly (Acrylamide-co-2-Acrylamido-2-methylpropane sulfonic acid). This matrix is loaded with reduced graphene oxide and nano particles of nickel oxide during the polymerization process. The resulting rGO@CMC-g-poly (AM-co-AMPS), NiO@CMC-g-poly(AM-co-AMPS) and NiO@rGO@CMC-g-poly(AM-co-AMPS) composite cryogels will be used as as solid electrolytes and super capacitors. The chemical composition, crystallinity, and morphological structure has been studied for those cryogels using FTIR, XRD, TGA and SEM-EDX. Cyclic voltammetry, galvanostatic charge-discharge rate and electrochemical impedance spectroscopy were used to determine the electrochemical performance of the prepared hydrogel samples.



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Hydrophobic ceramic capillary membranes applied for desalination by membrane distillation

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One of the potential methods for the treatment of saline water is Membrane Distillation (MD). MD is a thermally driven separation process where the driving force is the difference of partial pressure across the membrane, which is induced by the temperature difference applied on both sides of the membrane.[1] The feed solution is vaporized at the membrane interface, and the vapors pass through the membrane pores and condense on the cold side of the membrane as permeate.[2] Only porous hydrophobic membranes can be used in the MD process, as the surface should be non-wetting and allow only vapors to pass through the membrane pores.[3] Although polymeric membranes are widely studied in MD applications, ceramic membranes can be more advantageous due to their great mechanical strength, high chemical and thermal stability.[4]

In this work, we fabricated tubular ceramic support made of cordierite by extrusion process. The supports were prepared with different pore-forming agents like corn starch, rice husk, and maize flour. The surface of the support was coated with filtration layers of zirconia and γ-Alumina. Since the membrane had to be hydrophobic, the membrane surface was modified by grafting alkoxysilane groups containing 6, 8, and 12 carbon atoms in the alkyl chain. The filtration layers and the membrane morphology were observed by SEM; the structure and the orientation of the raw powders were analyzed by XRD, and the mechanical strength of the membrane was determined using the 3-point bending method. The pore size was calculated by Mercury Porosimetry and was found to be between 5 and 8 µm. The permeability of the hydrophilic membrane was between 1000 and 1500 L m^{-2} h^{-1} $bar^{-1,}$ and the Liquid Entry Pressure (LEP) of the modified hydrophobic membranes was between 2 and 6 bar. Later, MD in Air Gap configuration was performed using NaCl solution as the feed at a concentration of 0.5 M to yield an efficiency of 98 % of salt rejection for a temperature gradient of 80 °C.

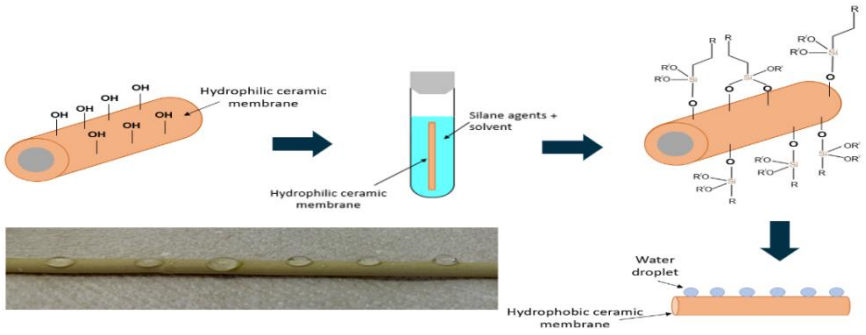

Figure: Chemical grafting of hydrophobic functional groups on the membrane.

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Mechanochemical ATRP: Practical conditions for liquid and solid monomers controlled polymerization in the ball mill

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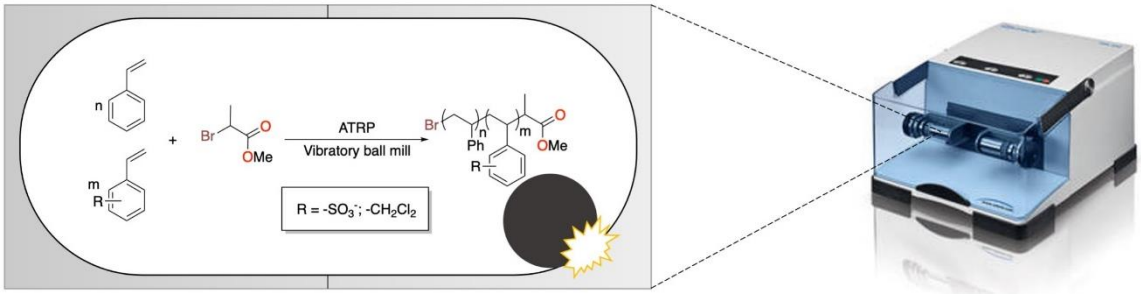
Discovered in 1995 by K. Matyjaszewski,[25] Atom Transfer Radical Polymerization (ATRP) is one breakthrough technique in the synthesis of polymers. Since its discovery, ATRP has been improved and became one of the most used techniques to produce well defined and controlled polymers unreachable otherwise. Nevertheless, there are still drawbacks to overcome such as the large amount of solvent, the time required to carry out the reaction or the impossibility to carry out reaction in pure aqueous media.[2] One way to overcome these drawbacks is mechanochemistry in a ball mill,[Erreur ! Source du renvoi introuvable.] an emerging branch of chemistry that allows the reaction to take place in the solid-state.[3] In 2020, H. Y. Cho and C. W. Bielawski described the first Activator ReGenerated by Electron Transfer (ARGET) ATRP of solid monomers by mechanochemistry in a ball mill resolving some of the drawbacks mentioned above.[5] Inspired by this work and to develop further ATRP in a ball-mill, we developed novel user-friendly conditions that allow the polymerization of liquid and/or solid monomers to form either polymers or copolymers.



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Design and Synthesis of Kallikrein 6 Inhibitors for Multiple Sclerosis Treatment

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Multiple sclerosis (MS) is a neurodegenerative and inflammatory disease affecting the peripheral and central nervous system causing lesions on the myelin sheath surrounding axons. The demyelination process causes severe motor, sensory and cognitive disorders, making MS the leading cause of non-traumatic disability among young adults. Kallikrein 6 (KLK6) is a serine protease produced by oligodendrocytes which was identified as a regulator of the myelin sheath volume.[1] While the overexpression of KLK6 leads to degeneration in the CNS, inhibiting its activity was proved efficient for limiting this latter effect and promoting remyelination, making this protein an interesting target for MS treatment.[2] Competitive and reversible inhibitors of the KLK6 were previously identified by our research group, based on the salicinamide motif.[3] These compounds proved to be non-toxic for cortical and striatal neurons and able to promote myelination *ex-vivo.* The presented work is aiming the optimization of these structures for increasing the enzyme-inhibiting properties of our previous hits, by using a structure-activity relationship-based strategy. Modulations of the amide, phenol and R_1 to R_3 groups were studied. Synthetic pathways and KLK6 inhibition results will be presented.

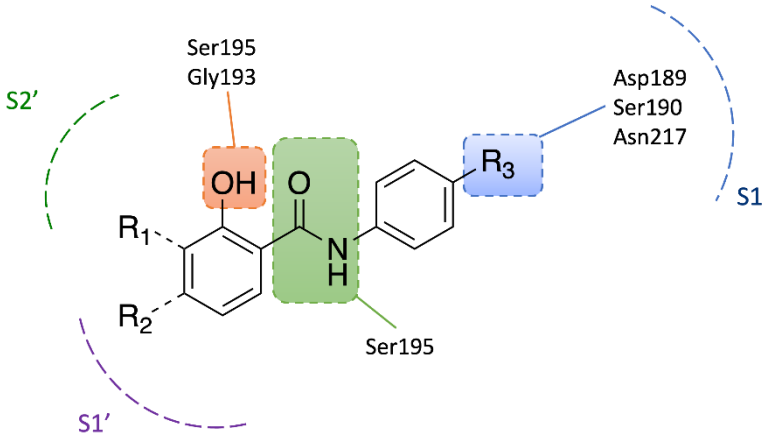

Figure: General structure of identified KLK6 inhibitors and key interactions predicted by docking in the enzyme's active site

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Solid-state chemistry shuffling of alkali ions towards new layered oxide materials

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The crystal structure of layered alkali transition metals oxides has focused the interest of the solid-state chemists as it offers a wonderful playground for chemical compositions and physical properties. The structure consists of stacking of transition metal layers with alkali elements sandwiched in between. While cationic substitutions in transition metal layers are well-studied, mixing different alkali elements is less explored. Thus, we undertook the solid-state exploration of the ternary system $Li_2Ni_2TeO_6$–$Na_2Ni_2TeO_6$–$K_2Ni_2TeO_6$, which all exhibit layered structures with alternating alkali cations and in-plane honeycomb ordering between nickel and tellurium.[1-3] A composition, $NaKNi_2TeO_6$, exhibiting a mixing of two alkali elements have already been reported. This is the first composition displaying an alternation of sodium and potassium layers.[4,5]

In our pursuit to extend the playground we have achieved the synthesis of novel alkali-mixed compositions featuring alternating stacking of two or even three different alkali cations, presenting a significant challenge in structural analysis, especially in localizing the alkali cations and identifying potential stacking defects. Our work combines various characterization techniques, such as diffraction methods (X-ray and neutron powder diffraction) revealing long-range alternation of alkali layers, and local analyses (high-resolution TEM and solid-state NMR) providing a detailed atomic-scale view. We have also explored the formation mechanisms, finding that synthesis occurs at moderate temperatures due to the high mobility of alkali cations, favoring a classical nucleation/growth process over simultaneous ionic exchange.

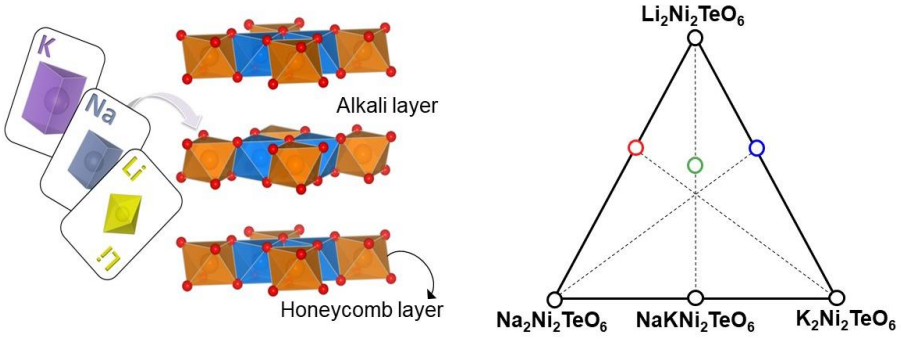

Figure: Crystal structure of the layered compounds $A_2Ni_2TeO_6$ (A = Li, Na, K) and the ternary phase diagram.

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Synthesis of zeolite A under sonohydrothermal conditions and investigation of its conversion into sodalite

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Keywords: Hydrothermal, Ultrasound, Sonohydrothermal; Zeolite A, Sodalite

Ultrasound is more and more used in many fields and in particular for the synthesis of nanomaterials. But for the moment only few stbeen conducted to understand the processes involved during the synthesis of nanomaterials in hydrothermal water under ultrasound, hence the novelty of the subject of study. We are interested in the synthesis of zeolite A and its conversion into sodalite under simultaneous action of hydrothermal conditions and 20 kHz ultrasound (SHT). To determine the impact of ultrasound on the kinetics of conversion of zeolite A into sodalite, different experiments were conducted starting from dissolved silica and sodium aluminate. First, the syntheses were carried out in conventional autoclave at 150 °C during 12 hours only conditions under which sodalite forms. Other syntheses were performed in the SHT reactor at 100°C for 30 minutes

After studying the impact of synthesis time and synthesis temperature on the conversion of LTA to sodalite in the SHT reactor and in hydrothermal synthesis, we investigated the influence of other parameters in the conversion of LTA into sodalite, such as the viscosity of the medium and the ratio Si/Na and Si/Al, the density and sound power absorbed in the reactor in the SHT reactor, the pressure in the Parr bomb reactor. After a precipitation under silent conditions, the samples were processed at 100 °C from 1 hour to 3 hours in the SHT reactor and 12 h at 150°C in the HT reactor respectively. The characterization of the products by scanning electron microscopy and by powder XRD revealed the impact of SHT treatment on the size and morphology of the crystalline products and also on the conversion kinetics of the amorphous gel into LTA and sodalite.

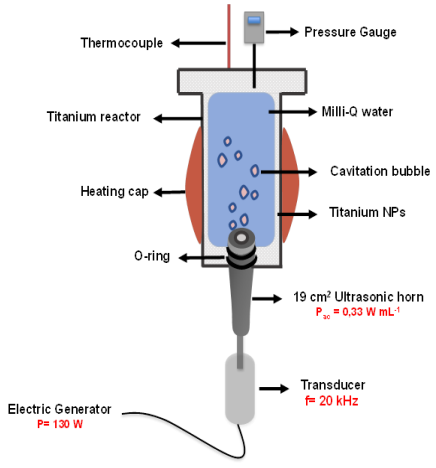
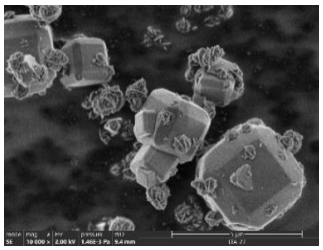
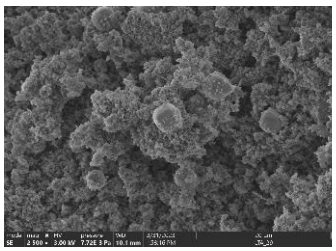


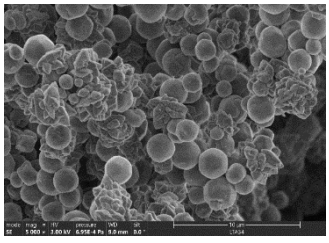
Figure : Sonohydrothermal reactor scheme



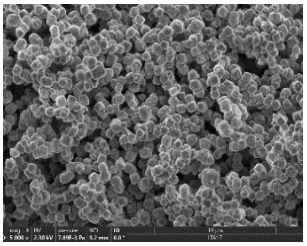
SHT(100°C/1H) 70% reactor filling rate



SHT(100°C/1H) 100% reactro filling rate



HT(150°C/12H) 70% bomb filling rate



SHT(100°C/3H) low densité

Amidation by reactive extrusion for the synthesis of active pharmaceutical ingredients teriflunomide and moclobemide

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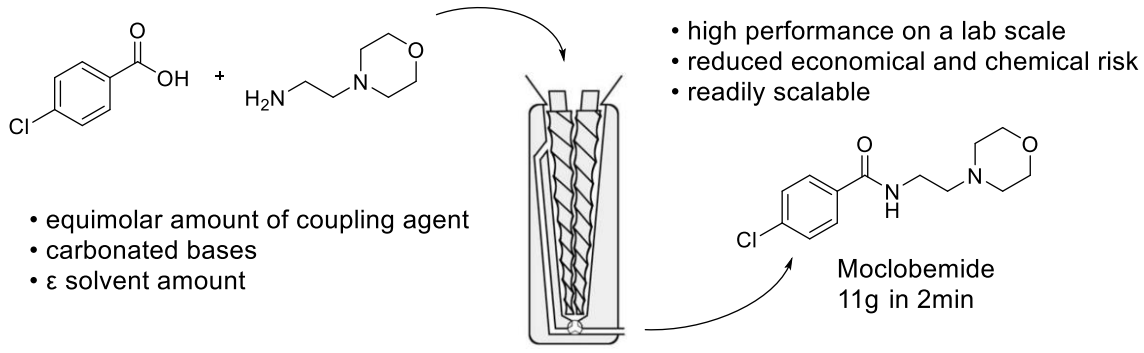
The pharmaceutical sector heavily relies on organic solvents, to produce active pharmaceutical ingredients (APIs). However, these solvents are frequently hazardous, toxic and environmentally harmful. To address the ecological and economic challenges associated with solvent usage in the fine chemicals industry, the Green Chemistry and Enabling Technologies team at IBMM has been engaged in developing mechanochemistry methods, primarily through ball-milling which allows for solventless reactions[1]. However, ball-milling is a batch process carried out in a closed reactor, and scaling up the reactions has proven to be challenging. A novel approach involved transitioning these processes into a continuous mode by employing an extruder, a conventional piece of equipment commonly used in polymer and food science, capable of handling solids or highly concentrated mixtures. This innovative method demonstrated its ability to efficiently form amide bonds[2], a critical component in 25% of the drugs available on the market. An innovative approach allowing the production of an amide, from the inactivated acid and amine moieties will be presented. This method was applied to the synthesis of two essential APIs: teriflunomide, used in the treatment of multiple sclerosis, and moclobemide, an antidepressant. Remarkably, this continuous process enabled the synthesis of 11 grams of moclobemide in just 2 minutes, and by simply replenishing the raw materials, the desired quantity could be readily produced. The potential impact of these findings on the pharmaceutical industry is already evident[3].



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Tuning transmembrane transport by playing with C-H donor strength in a series of bis(cyanostilbene) podants

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The transmembrane transport of physiologically relevant species is a fundamental process in living organisms. Although Nature has exquisitely designed specialized proteins to modulate (actively or passively, and in most cases with an impressive selectivity) the ion/molecular trafficking along phospholipid bilayer, the idea of artificial transporters (channels and carriers) came as an innovative solution to biomimic the natural functions in order to overcome the processability, stability and scalability issues imposed by natural channels. Thus, artificial transporters opened the gate toward a myriad of applications in many biological areas, as well as in separation, signaling and delivery processes. Among these, perhaps the most important achievements are the overcoming of permeability/selectivity trade-off in water desalination processes by using artificial water channels (AWCs),[1] and apoptosis induced in cancer cells by artificial anion channels/carriers.[2]

Within this appealing context, we disclose here a finely tailored series of simple and easily accessible small cyanostilbene-based bipodants (Figure 1) which are able to self-stack in channel-like architectures and to facilitate the water and/or anion translocation along membrane bilayer. The variation of C-H donor strength allowed us to fine-tune the selectivity of these synthetic transporters. For example, **CH-3**, having the less acidic protons, does not translocate ions but transports water efficiently. Therefore, it is a good candidate for water desalination. On the other hand, **CH-1**, **CH-2**, **CH-4** and **CH-5** sustain the electrogenic uniport of NO_3^-, Br^- and Cl^- in this order of selectivity. Interestingly, **CH-6** is completely selective for nitrate. This selectivity order (i.e., NO_3^- >> Br^- > Cl^-) is in sharp contrast with the selectivity order of N-H donor analogous.[2,3] Thus, our study provides valuable insights into the correlation between structure, recognition ability, transporter-solute interaction strength and transport activity, paving the way toward a rational design of artificial channels/carriers with boosted properties and targeted applications.

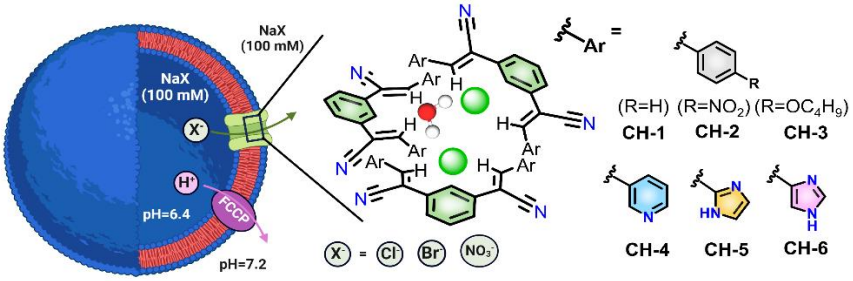

*Figure: Water-mediated electrogenic uniport of different anions (Cl^-, Br^-, NO_3^-) across lipid bilayer facilitated by channels assembled by **CH-1-6** in synergy with FCCP – a proton carrier.*

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Selective Water Pore Recognition and Transport through Self-Assembled Alkyl-Ureido-Trianglamine Artificial Water Channels

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Keywords: charge transport, membranes, molecules, permeability, vesicles

In nature, aquaporins (AQPs) are proteins known for fast water transport through the membrane of living cells. Artificial water channels (AWCs) synthetic counterparts with intrinsic water permeability have been developed with the hope of mimicking the performances and the natural functions of AQPs. Highly selective AWCs are needed, and the design of selectivity filters for water is of tremendous importance. Herein, we report the use of self-assembled trianglamine macrocycles acting as AWCs in lipid bilayer membranes that are able to transport water with steric restriction along biomimetic H-bonding-decorated pores conferring selective binding filters for water. Trianglamine [(±)Δ, (mixture of diastereoisomers) and (R,R)3Δ and (S,S)3Δ], trianglamine hydrochloride (Δ.HCl), and alkyl-ureido trianglamines (*n* = 4, 6, 8, and 12) [(±)ΔC4, (±)ΔC8, (±)ΔC6, and (±)ΔC12] were synthesized for the studies presented here. The single-crystal X-ray structures confirmed that trianglamines form a tubular superstructure in the solid state. The water translocation is controlled via successive selective H-bonding pores (a diameter of 3 Å) and highly permeable hydrophobic vestibules (a diameter of 5 Å). The self-assembled alkyl-ureido-trianglamines achieve a single-channel permeability of 108 water molecules/second/channel, which is within 1 order of magnitude lower than AQPs with good ability to sterically reject ions and preventing the proton transport. Trianglamines present potential for engineering membranes for water purification and separation technologies.

Chiral biaryls: from axial to planar chirality using Kumada-Tamao-Corriu coupling

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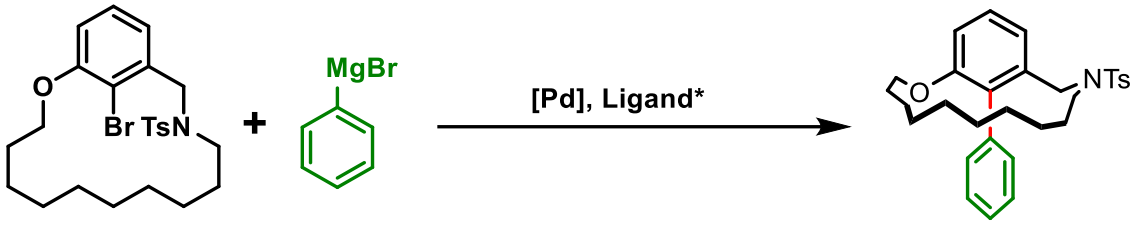
Palladium- or nickel-catalyzed Kumada-Tamao-Corriu couplings are widely used to synthetize biaryl compounds. Several ligands have been tested to develop enantioselective versions giving access to biaryls containing an axis of chirality.[1] Whereas good enantiomeric excesses can be obtained with including phosphorus-based chiral ligands, enantioinduction using chiral N-heterocyclic carbenes (NHC) is rather moderate, including with atropisomeric Pd-NHC complexes recently develop in our laboratory.[2,3] This led us to investigate this coupling reaction with peculiar substrates for which a planar chirality will be generated instead of an axial chirality: cyclophanes.

Cyclophanes are macrocycles composed from an aromatic ring and an *ansa* chain and can be found in many natural and pharmaceutical compounds.[4] Para- or metacyclophanes can display a planar chirality but methods to prepare them in an enantioenriched manner are limited, especially for metacyclophanes. In this work, it will be presented the synthesis of metacyclophanes, the study of their configurational stability and their uses in the Kumada-Tamao-Corriu coupling to generate enantioenriched planar chiral biaryls metacyclophanes with up to good ees (88% ee).



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Structural study of piezoelectric $LnCa_4O(BO_3)_3$ at high pressures and cryogenic temperatures

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In spite of their small piezoelectric effect, quartz crystals continue to dominate as components for frequency control since the early days of radio engineering, due to their extremely sharp resonance curves, which are stable with respect to temperature and aging. Lanthanide oxyborate crystals, *Ln*COB ($LnCa_4O(BO_3)_3$ with *Ln* = *La* to *Yb* is found to be quite attractive as they exhibit excellent piezoelectric properties more than three times that of quartz in a large temperature range (300≤T ≤1000°C). However up to now, they were not investigated either at cryogenic temperatures and/or under high-pressure in spite of important concern in piezoelectric application in orbit and LT/HP-sensors. This is therefore the aim of the present study.

Ln-oxyborates crystallise in the monoclinic *Cm* space group which was found to be stable from our DFT-calculations. *Ln*- and *Ca*-ions exhibit distorted edge-shared octahedra connected by BO_3 groups along c*, ***Fig a***. Optimal piezoelectric properties were found to be linked to the *Ln*-ion radius (best for rLn^{3+} similar to rCa^{2+}). High quality single crystals [1] have been characterized in house using 4-circle Bruker D8 diffractometer using Mo K_α-radiation in the 100 ≤ *T* ≤ 350K temperature range. Additionally, *Nd* and *Er*-based oxyborate crystals were studied at high pressure (1 ≤ *P* ≤ 6 GPa) and low temperature (10-300 K) using single crystal X-ray diffraction at the XPRESS beamline at ELETTRA synchrotron using 0.5 Å wavelength photons and PILATUS 3S 6M detector. High-pressure experiments were conducted using a diamond anvil cell using helium as pressure transmitting medium.

Whereas *Nd*COB was found to keep the *Cm* monoclinic structure in the 100-350K temperature range, *La*COB transformed below 150K into an incommensurate structure, ***Fig b***. Additionally, *Er*COB and *Tm*COB were found to exhibit (Ca/Ln) site disorder, ***Fig c,*** which could explain the observed lower piezoelectric properties [1].

Cryogenic structural characterization under high pressure led to a similar incommensurate transition of *Nd*COB to that previously determined for *La*COB below 30K in the entire pressure range. However, such a transformation was absent for *Er*COB, probably due to the site-disorder previously described. These structural characterizations have now to be compared with on-going cryogenic temperatures and/or under high-pressure piezoelectric measurements.

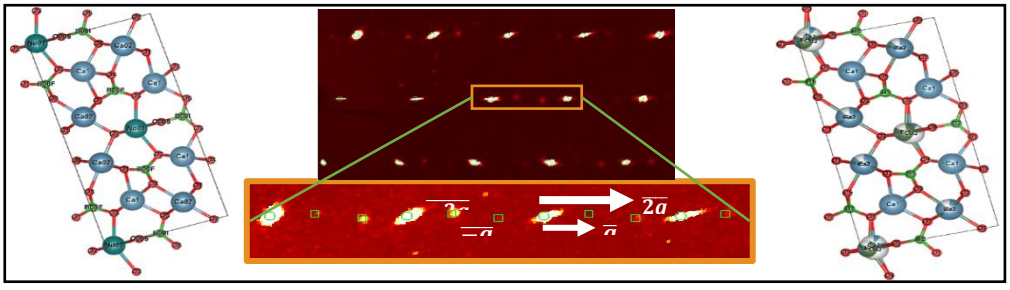

Figure: Cm monoclinic structure of NdCOB, **b)** hk0 reconstruction of the reciprocal space showing the appearance of satellites for $\bar{q}$=0.625a*+0.01c*, **c)** site-disorder characterized for ErCOB (R_1=2.9%)

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○ 6 Posters

ll Celeste SOUCHE - IBMM, Montpellier.
“In-depth study of the 68Ga radiolabeling conditions of a bisphosphonate monoamide analog of DOTA for bone imaging”

ll Maximilien CORONAS – IEM, Montpellier.
“Self-assembly of polymeric membrane and introduction of inorganic compounds”

ll Jordan LEHOUX – IBMM, Montpellier.
“Lipophenols: Synthesis and applications as both analytical standards and therapeutic derivatives”

ll Ludivine ONILLON – ICGM, Montpellier.
“Bio-Sourced Ionic Aerogels from Hydrothermal Carbonization”

ll Karen MENGUE ME NDONG – ICGM, Montpellier.
“Hydrophosphonylation of Coumarins and Isophosphinoline 2-oxides”

ll Ludivine POYAC – ICGM, Montpellier.
“Electronic, steric and catalytic properties of N-heterocyclic carbene rhodium(I) complexes linked to (metallo)porphyrins”