UNIVERSITÉ DE NAMUR

Women and Girls in Science Day

WOMEN & GIRLS IN SCIENCE

UNIVERSITÉ DE NAMUR

Book of abstracts

2026

12th February 2026 | 6th edition

Women and Girls in Science

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Our 2026 event is supported by

Women and Girls in Science

Programme 2026

08:30	**Welcome, coffee breakfast and registration**
09:15	**Welcome words**
09:25 – Keynote 1	**Prof. Nelly Litvak** - Eindhoven University of Technology, Mathematics and Computer Science
10:15 – Talk 1	**Dr. Shalini Iyer -** UNamur, Faculty of Science, Department of Physics, NARILIS Research Institute
10:35	**10:35 – Coffee break**
11:05 – Talk 2	**Prof. Serena Silvi** - University of Bologna, Department of Chemistry
11:25 – Talk 3	**Dr. Manel Barkallah** - UNamur, Faculty of Computer Science, NaDI Research Institute
11:45 – Talk 4	**Prof. Liselot Dewachter**, UCL, de Duve Institute
12:05	**Flash talks**
13:00	**Lunch and Poster Session**
14:30 – Keynote 2	**Prof. Roosmarijn Vandenbroucke - UGent, Human diseases: Immunology & inflammation**
15:20 – Talk 5	**Prof. Mercedes Alonso Giner** - Vrije Universiteit Brussel (VUB), Department of General Chemistry, Algemene Chemie (ALGC)
15:40	**Coffee break**
16:10 – Talk 6	**Prof. Elsa Roland** - UNamur, Faculty of Education and Training Sciences, IRDENa Research Institute
16:30 – Panel session	**Featuring former committee members: sharing experiences, insights, and perspectives on advancing women's roles in science**
17:30	**Closing remarks and prizes**
18:00	**Drink and networking**

Awards and prizes by Fonds Adrien Bauchau

A total of four awards will be presented, with one audience award and one jury award for Flash Talks, and one audience award and one jury award for Posters.

The prize for each award will be 250€.

250 € each

- **Best Flash talk: Audience and jury awards**
- **Best Poster: Audience and jury awards**

The Fund was created in memory of Adrien Bauchau. The Adrien Bauchau Fund (FAB) promotes excellence in education and research in the life sciences. Its primary base is at the University of Namur (French Community of Belgium). The FAB's regular activities (annual or biennial) within the Belgian university context include: awarding scholarships, prizes, and grants; establishing a chair; and contributing to the organization of conferences, doctoral schools, and study days.

The FAB sought to demonstrate its commitment to the University of Namur community by creating the "Espace Bauchau." Located at the junction of the Medicine and Cellular and Molecular Biology buildings with the Organismal Biology building, it offers students a welcoming and peaceful space. A selection of journals is available, and display cases showcase examples of major discoveries in biology. By creating a Training and Development branch in 2005, the FAB expanded its activities to include training students and promoting researchers from developing countries.

It collaborates with a network of Belgian and international partners: individuals, public and private associations, institutions, and businesses. The FAB benefits from the human and financial support of numerous university alumni (ABAN: Association of Former Biologists of Namur) as well as the patronage of the Bauchau family and other supportive families and individuals.

Welcome to Women and Girls in Science Day

The International Day of Women and Girls in Science takes place every 11th of February, following the declaration by the General Assembly of the United Nations on 22nd of December 2015. This annual event aims at promoting the access of women and girls to science and technology as well as their full and fair participation. It reminds the important role of women in the scientific community and constitutes a great opportunity to encourage girls and young women to participate in the scientific developments.

The 6th edition of Women and Girls in Science Day will take place on February 12, 2026, at Rosalin Franklin Auditorium at the Faculty of Science of the University of Namur.

This year, the official Opening will be delivered by Anne-Catherine Heuskin, professor at physics department in University of Namur

Keynotes speakers

Keynote 1

Prof. Nelly Litvak
Eindhoven University of Technology, Mathematics and Computer Science

Image Credit: < Angeline Swinkels >

Prof. Nelly Litvak is professor in Algorithms for Complex Networks and has a background in Applied Probability and Stochastic Operations Research. She works on mathematical methods and algorithms for complex networks, such as social networks and the WWW. Real-life networks are modeled as random graphs, and algorithms are used to extract information from the massive network data.

The overall goal of her research is to extract value from (Big) Data, focusing on network data. Her research revolves around three main topics: Information extraction and predictions based on data, mathematical analysis of network characteristics and randomized algorithms. The first looks at defining and collecting the correct measurements and data for specific purposes and deducing networks from data. The second examines mathematical properties of algorithms in networks, for example, the famous PageRank that Google invented to rank web pages. The third looks at efficient algorithms for computing network characteristics when the complete network data is not available.

Learning the growth mechanisms of citation networks

Real-life complex networks, such as social networks, world wide web and the network of scientific citations, often have a so-called scale-free property. It means that there is a small number of nodes with exceptionally large number of connections. The Preferential Attachment mechanism says that highly-cited papers can be expected to get even more citations, thus giving rise to a rich-get-richer effect and scale-free property. This model for citation networks was proposed as early as 1965 by De Solla Price and is often put forward in the literature as a main driver for the emergence of the scale-free property. Besides Preferential Attachment, however, the state-of-the-art models for citation networks include other mechanisms, such as fitness (good papers cited more) and ageing (old papers

are cited less). The question remains, which of these mechanisms are truly behind the network formation, and which are just plausible models?

In this talk, I will first introduce the scale-free property and show how it is derived from the Preferential Attachment mechanism. Then I will describe our model-selection method that aims to identify which combination of growth mechanisms is the best fit for the real-life citation networks. This method involves training a classifier on a large body of synthetic networks. We design a conceptually novel type of dynamic features that count new citations received by a group of papers in a particular time interval. The proposed features are easy to compute and are interpretable. Our approach achieves a near-perfect classification of synthetic networks, exceeding the state-of-the-art by a large margin. Applying our classification method to real-world citation networks gives credibility to the state-of-the-art models but also shows that some plausible mechanisms are not always confirmed by the data.

Keynote 2

Prof. Roosmarijn Vandenbroucke
UGent, Human diseases: Immunology & inflammation

Prof. Roosmarijn Vandenbroucke was born in 1979 in Izegem. She graduated in biotechnology in 2001 and began her academic journey as a doctoral student at the General Biochemistry laboratory at Ghent University, culminating in the completion of her doctoral studies in Pharmaceutical Sciences in 2008. Her dissertation focused on non-viral nucleic acid delivery systems. She then began a postdoctoral research period on sepsis, supported by a grant from the Flemish Funding Agency (FWO).

Roosmarijn is head of the Barriers in Inflammation at the VIB-UGent Center for Inflammation Research (Ghent, Belgium). She has a background in biotechnology and molecular cell biology. She obtained a PhD in Pharmaceutical Sciences at Ghent University (Belgium) where she focused on gene therapy. During her postdoctoral research, she became interested in peripheral and central inflammation and brain barriers. She founded her independent research lab at Ghent University in 2015 and at VIB in 2018. Her team is internationally recognized for its expertise in brain barriers, (neuro)inflammation, the gut-brain axis, and extracellular vesicles.

Signaling and immune surveillance at the choroid plexus in CNS disease

The choroid plexus (ChP) has emerged as a dynamic neuroimmune interface that integrates signals from the periphery to regulate central nervous system (CNS) homeostasis. Research in the Barriers in Inflammation lab focuses on how the ChP decodes peripheral inflammatory cues and relay them to the brain through altered barrier function, cytokine signaling, and extracellular vesicle (EV) communication. We investigate how systemic inflammation reshapes ChP-mediated immune surveillance, influencing both the recruitment and phenotypic modulation of immune cells trafficking into the CNS. These mechanisms are increasingly implicated in neurodegenerative disorders, including Alzheimer's disease, where ChP dysfunction, chronic inflammation, and immune cell trafficking converge to accelerate disease progression. By dissecting these interconnected pathways, our research aims to unravel how ChP–immune crosstalk contributes to CNS pathology and to identify novel therapeutic entry points targeting the blood–brain–CSF interface.

Short talk speakers

Talk 1

Dr. Shalini Iyer
University of Namur (Faculty of Science, Department of Physics)

Dr. Shalini Iyer is a post-doctoral researcher in the Faculty of Science, Department of Physics at the University of Namur. She did an interdisciplinary PhD at UNamur where she created gold nanoparticles that could improve the anti-cancer immune response after X-ray and proton therapy. Shalini's current work involves pre-clinical research to assess the translation of this treatment approach.

Under-representation of women in clinical trials

Women remain under-represented in clinical trials despite comprising roughly half of the patient population. This disparity is particularly evident in early-phase trials and studies of cardiovascular and pharmacological interventions. This has significant clinical and scientific consequences, including increased adverse drug reactions, inaccurate dosing, delayed diagnosis of disease patterns, and reduced generalizability of study findings. Approaches to improve this disproportion include sex-balanced recruitment, inclusive eligibility criteria, flexible trial logistics, and greater female representation in trial leadership, ultimately improving the safety, efficacy, and equity of medical interventions.

Talk 2

Prof. Serena Silvi
UNamur (Faculty of Science, Department of Physics)

Prof. Serena Silvi is Associate Professor at the Chemistry Department "Giacomo Ciamician," University of Bologna, where she studies the photophysical, photochemical, and electrochemical properties of supramolecular systems. Her research focuses on the design and characterization of artificial molecular machines and complex systems for signal processing.

She earned her Laurea in Chemistry cum laude from the University of Bologna in 2002 under Prof. Vincenzo Balzani, with a thesis on novel prototypes of artificial molecular machines. She completed her Ph.D. in Chemical Sciences in 2006 under the supervision of Prof. Alberto Credi, with a dissertation entitled "Artificial Molecular Machines", including a six-month research stay in Prof. Angel E. Kaifer's laboratory at the University of Miami.

From 2006 to 2008, she collaborated in the Photochemistry and Supramolecular Chemistry Laboratory led by Prof. Balzani. Since 2008, she has been a researcher at the University of Bologna and qualified as Associate Professor in 2013 and 2018. She has authored over 80 publications, several book chapters, a European patent, and has edited volumes on photochemistry and molecular machines.

Designing artificial molecular machines

Movement is one of life's central attributes: indeed, Nature provides living systems with motor proteins, complex molecules that convert chemical energy into power to perform tasks, working like ordinary machines built for everyday needs. Thousands of different nanomachines operate within our bodies, enabling us to speak, see, walk, think. These biological engines, though, are not shrunk versions of their macroscopic counterparts, as they obey to distinct constraints, as a consequence of their dimensions. Indeed, molecular machines are soft and not rigid, they operate at near-ambient temperature, under conditions of high viscosity, and they are governed by noncovalent interactions. Moreover, they function far from equilibrium, manipulating their constant, random (Brownian) motion via ratcheting mechanisms to obtain controlled movements.

Here we will present how to design artificial molecular devices, taking into account the lessons learnt from biology and bearing in mind the marked difference between the operation mechanisms at the macroscopic and molecular level. Though artificial molecular machines cannot reproduce the structural and functional complexity of biomachines, nevertheless we can construct simple prototypes made of few molecular components, but using a larger chemical toolbox and operating in a wider range of conditions

Talk 3

Dr. Manel Barkallah
University of Namur (Faculty of Computer Science)

Dr. Manel Barkallah is a post-doctoral researcher at the Faculty of Computer Science of the University of Namur and a member of the NaDI (Namur Digital Institute) research institute. She works on Formal Methods for Coordination Languages. During her PhD, she developed Anemone, a framework based on coordination models and automata-based techniques to address complex distributed scenarios such as smart cities and IoT systems.

In her current postdoctoral work, she continues this research line by applying lightweight formal methods to cybersecurity. Within the CyberExcellence project, funded by the Walloon Region of Belgium, her work aims analysing, modelling, and improving the correctness and robustness of security protocols.

A lightweight approach to coordination and formal method

Modern technologies such as smart cities, IoT systems, and connected environments rely on many components acting at the same time and interacting with each other. Understanding and controlling these concurrent behaviours is essential, yet it remains a difficult task, even for experts. While formal methods offer powerful tools to reason about such systems, they are often perceived as too complex and therefore remain underused in practice.

In this talk, I will present the Anemone Workbench, a lightweight and accessible framework designed to make concurrency easier to understand, explore, and analyse. Anemone combines a coordination language inspired by shared data spaces with simple logical rules to describe how components interact over time. Rather than focusing on heavy mathematical formalisms, the approach emphasizes intuition, visualization, and executability. Through three illustrative examples -- a smart garden, a dynamic sports simulation, and a role-playing game -- I will show how complex concurrent behaviours can be modelled, animated, and reasoned about in an intuitive way. I will conclude by discussing how such lightweight formal methods can support education, early-stage system design, and interdisciplinary collaboration, while serving as a gateway toward more rigorous verification techniques.

Talk 4

Prof. Liselot Dewachter
Université Catholique de Louvain and de Duve Institute

Prof. Liselot Dewachter is a research associate of the FNRS and a professor at UCLouvain and the de Duve institute in Brussels, Belgium. Her team studies the fundamental cell biology of the bacterium Streptococcus pneumoniae in the hopes of discovering novel ways to kill this major human pathogen. Current research aims to better characterize how S. pneumoniae regulates crucial cell cycle processes (such as DNA replication, cell division, etc.) and characterizing these regulatory mechanisms at the molecular leve

Reverting antibiotic resistance to fight Streptococcus pneumoniae infection

Antibiotic resistance in the important human pathogen Streptococcus pneumoniae is on the rise. This is particularly problematic in the case of beta-lactam antibiotic amoxicillin, which is the first-line therapy against this bacterium. It is therefore crucial to uncover targets that would kill or re-sensitize amoxicillin-resistant pneumococci. To do so, we developed a genetic screening approach that combines CRISPR interference with cell sorting (CRISPRi-FACS-seq). Since amoxicillin affects growth and division, CRISPRi-FACS-seq was used to identify targets that are responsible for maintaining proper cell size. Our screen revealed that downregulation of the synthesis of bactoprenol, an important lipid carrier molecule, leads to extensive cell elongation. We successfully exploited this knowledge to create a combination treatment strategy where the FDA-approved drug clomiphene, an inhibitor of bactoprenol synthesis, is paired up with amoxicillin. Our results show that clomiphene potentiates the antimicrobial activity of amoxicillin and that combination therapy re-sensitizes amoxicillin-resistant S. pneumoniae. These findings could provide a starting point to develop a solution for the increasing amount of hard-to-treat amoxicillin-resistant pneumococcal infections.

Talk 5

Prof. Mercedes Alonso Giner
Vrije Universiteit Brussel , VUB (General chemistry research group)

Prof. Mercedes Alonso Giner is an assistant professor and postdoctoral associate funded by the FWO at the VUB. Her research exploits modern computational tools and conceptual methods towards the understanding and prediction of new organic or inorganic molecules as well as the design of sustainable chemical processes.

Accelerating Chemical Discovery through Computational Chemistry

Computational chemistry is reshaping how chemical discoveries are made by enabling rapid prediction, design, and optimization of molecules and materials. In this talk, I will show how modern computational tools—from quantum chemical simulations, inverse design to machine learning models— empower scientists to explore vast chemical spaces, accelerate discovery, and identify new functional compounds with targeted properties. Central to our approach is the integration of fundamental chemical concepts as guiding design principles to understand and navigate complex structure–property relationships.

Talk 6

Prof. Elsa Roland
University of Namur (Faculty of Education and Training Sciences)

Elsa Roland is a lecturer at the University of Namur and co-president of IRDENa. His research explores the history and political philosophy of education, with a particular interest in relationships of school and educational domination, their genealogies and their updates, both in the Wallonia-Brussels Federation and at the international level.

On the Emotional

This communication proposes a critical reflection on the links between gender, education and science. Based on research in educational sciences and the history of teaching, it questions an often-accepted fact: the neutrality of the school and the university. Gender is not considered as a simple variable of equality, but as a key to understanding pedagogical gestures, educational standards and academic careers. From childhood to scientific excellence, the presentation highlights the way in which educational institutions produce – but can also transform – gendered power relations.

Panel session

Featuring former committee members: sharing experiences, insights, and perspectives on advancing women's roles in science

Moderator

Dr. Aishwarya Saxena

Panelists

Prof. Liselot Dewachter

Prof. Anne-Catherine Heuskin

Dr. Manel Barkallah

Dr. Hala Kasmo

Flash Talks

Flash	Name	Title
1	Noémie Buratto	WHEN JELLYFISH WAKE UP: ENDOGENOUS DIURNAL RHYTHM AND INTER-INDIVIDUAL VARIABILITY IN PULSATION OF THE SYMBIOTIC JELLYFISH CASSIOPEA
2	Francesca Carlon	Thinking Like a Scientist? A Structural Study of LLM-Generated Research Methods
3	Chloé Célis	Preparation of novel bifunctional dendritic shaped nanoparticles for efficient CO2 valorization
4	Alexandra Dache	A Matrix Factorization Framework for Community Detection under the Degree-Corrected Block Model
5	Julie Dullier	Study of The Inhibition of LDH by Covalent SuFEx Inhibitors
6	Komlan Fiagbe	Avalanche size distributions in sandpile model on complex networks
7	Marine LEFEVRE	Bioorthogonal Pd-Catalyzed Anticancer Prodrug Activation: When Chemistry Drives Cytotoxicity
8	Aylin Melan	Shine Bright Like a Diamond - Even Under Stress: Modeling Spectral Shifts of Strained Color Centers
9	Driélle Müller	Eco-Friendly Aqueous Processing of NMC Cathodes for Next-Generation Li-Ion Batteries
10	TASNEEM OSMAN	From Invasive Plants to Disease Risk: An Overlooked One Health Perspective
11	Claudia Schrauwen	Multimodal Imaging Biomarkers of Lesion Severity and Functional Outcome in a Rat Model of Cervical Spinal Cord Injury
12	Laura Willam	The Joint Effect of Stressor Diversity and Biodiversity on Ecosystem Function in Algal Communities
13	Laura Zeidler	Can You Be More Explicit? A Task and Dataset on Explicitations of Implicit Meaning
14	Laurence Theunis	HeR-Lab, des actions RH innovantes pour booster la carrière des femmes dans la Tech

Posters

Poster	Name	Title
1	Marthe Ballon	Benchmarks Saturate When The Model Gets Smarter Than The Judge
2	Marion Bauwens	Insight into the processing mechanism of secreted bacterial intein-like domains
3	Emma Calluy	Association of frailty and sarcopenia with amyloid positivity
4	Lucie Caramelle	Drugging the Endoplasmic Reticulum Exit Sites (ERES)
5	Ines de Fays	ERES, GATOR2 and NPC: Is complex activity determined by Sec13?
6	Nicole Goede	Embryos at risk: Early embryonic development of aquatic ectotherms in a warming and polluted world
7	Verónica González	Towards reconstituting meiotic crossover formation
8	Sophie Van Heden	Towards a core outcome set for sarcopenia intervention studies: results from a Delphi study
9	Saima Kamaal	Development of Multi-Layered and Small-Molecule Biomimetics of Lytic Polysaccharide Monooxygenases Using Histidine Brace
10	Anita Kundu	Crystallisation and structural studies of 4-aminopyridine (4-AP) salt derivatives and 1-H imidazolium chloride
11	Médéa Locquet	Cancer-treatment-induced biological and epigenetic signs of accelerated aging in cancer survivors: A systematic review
12	Lorien Macenulty	How the scientific masculinity can help us deconstruct barriers to recruitment and retention of gender minorities in STEM
13	Manon Mirgaux	AI-guided competitive docking for virtual screening and compound efficacy prediction
14	Keïla OPELE-NAVENGE	Targeting ferroptosis resistance to sensitise cancer cells to radiotherapy/protontherapy
15	Lakshmi Narayan Satheesh Babu	Iron Based Photosensitizers Anchored on Metal Oxide Thin Films for a Greener Future
16	Jozie Tientcheu	Synthesis of new beta-lactams analogues designed for the detection of antimicrobial bacterial resistance by electrochemistry
17	Alessia Tonelli	SYNTHESIS OF CARBON-BASED BIFUNCTIONAL LEWIS/BRÃ˜NSTED ACID CATALYSTS FOR 5-HMF PRODUCTION FROM CELLOBIOSE
18	Marie Rose YOUBI KEMMOGNE	Active-learning guide force-field development for NMC cathode modeling

Flash Talks Abstracts

WHEN JELLYFISH WAKE UP: ENDOGENOUS DIURNAL RHYTHM AND INTER-INDIVIDUAL VARIABILITY IN PULSATION OF THE SYMBIOTIC JELLYFISH *CASSIOPEA*

Noémie BURATTO [1*], Eli THORÉ [1,2,3]

[1] Laboratory of Adaptive Biodynamics, Research Unit in Environmental and Evolutionary Biology (Department of Biology), Institute of Life, Earth, and Environment, University of Namur, Rue de Bruxelles 61, 5000 Namur, Belgium.

[2] Department of Wildlife, Fish, and Environmental Studies, Swedish University of Agricultural Sciences, Skogsmarksgränd 17, 907–36 Umeå, Sweden.

[3] TRANSfarm, Science, Engineering, and Technology Group, KU Leuven, Bijzondereweg 12, 3360 Bierbeek, Belgium.

***Presenting author**, noemie.buratto@unamur.be

Keywords: *Cassiopea* spp., diurnal rythm, pulsation behavior, symbiosis.

Benthic jellyfish of the genus *Cassiopea* exhibit regular pulsatile behavior that makes them an original model for studying behavioral rhythms in photosymbiotic cnidarians. This pulsation, essential for water circulation and gas exchange, serves as a reliable indicator of physiological state. Easily measurable, it provides a rare opportunity to experimentally study behavior in organisms lacking a centralized nervous system. Previous studies have also revealed in *Cassiopea* a nocturnal quiescent state comparable to sleep, suggesting circadian regulation of activity. However, the fine dynamics of this cycle have remained largely undescribed.

We monitored the pulsation frequency of 30 *Cassiopea* spp. individuals from a natural population over 72 hours, at four key moments of the nycthemeral cycle: dawn, noon, dusk, and midnight. The jellyfish were maintained under natural light and temperature conditions. The analysis reveals a marked rhythm, with a clear activity peak at dawn (≈ +17% compared to the mean) and a pronounced minimum at midnight. Bell diameter negatively influences pulsation frequency, but more than 60% of the total variance remains due to interindividual differences independent of size, indicating that each jellyfish maintains its own rhythm.

The morning peak, observed without feeding, precedes light intensification and reflects anticipatory activation consistent with endogenous control. These results suggest that pulsatile activity, rather than a direct response to photosymbiosis, reflects an autonomous rhythm anchored in physiology. *Cassiopea* thus stands out as a privileged model for exploring the links between biological rhythms, symbiosis, and emerging behaviors in early animal lineages.

Thinking Like a Scientist? A Structural Study of LLM-Generated Research Methods

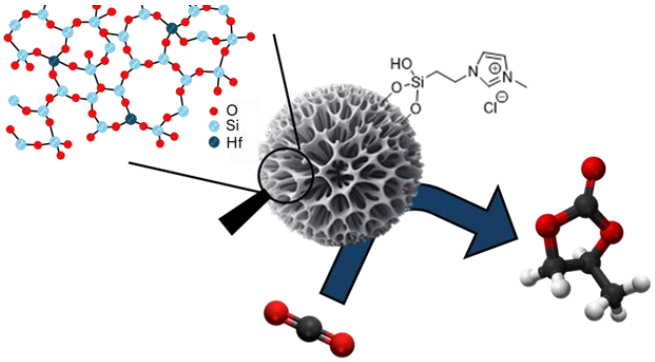
Francesca Carlon, Vincent Ginis, Andres Algaba
Data Analytics Lab, Vrije Universiteit Brussel (VUB)
francesca.carlon@vub.be

The scientific community has significantly benefited from the integration of artificial intelligence, especially large language models (LLMs), into academic research. These tools support not only idea generation and literature review but also suggest methodologies and experimental designs, thereby accelerating the entire research pipeline. However, the implications of relying on LLM-generated guidance, particularly regarding potential biases or preferences, remain underexplored. Here, we investigate the nature and consistency of methodological suggestions provided by different LLMs in the context of AI research. Specifically, we compare the ground truth choices on the datasets, models, and evaluation metrics with LLM-generated suggestions in response to research questions derived from published AI papers. With this experiment, we aim to uncover patterns, biases, or preferences in how LLMs approach research design. Insights from this analysis may inform researchers about the reliability and limits of using LLMs as methodological advisors.

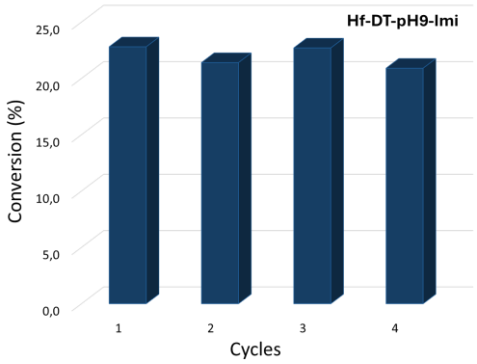
Preparation of novel bifunctional dendritic shaped nanoparticles for efficient CO_2 valorization

Chloé Célis, Nicolas Pierard, Anthony Morena, Carmela Aprile
Laboratory, Department, University CMA Lab, CNANO Unit, Chemistry Department, University of Namur
chloe.celis@unamur.be

In the context of green chemistry, the conversion of CO_2 into value-added products, such as cyclic carbonates (CC), is particularly attractive for the valorization of this waste. However, the high stability of CO_2 requires the use of a catalyst, such as imidazolium organic salts often used in homogeneous phase[1]. Those compounds can be grafted on a solid support to obtain sustainable heterogeneous catalysts. These materials present the advantage of being easily reused, but are often less efficient due to diffusion limitation. In the field of heterogeneous catalysts, mesoporous silica-based materials are among the most investigated class of solids[2]. This is due to their interesting properties such as high pore volume and specific surface area, tunable pore size, thermal stability, mechanical robustness and the possibility to functionalize the surface. Moreover, in such materials, the insertion of suitable metal cations in the silica framework can provide both Brønsted and Lewis acid sites that act as co-catalysts in the conversion of CO_2 to CC. For example, hafnium atoms have already proven their efficiency for this reaction, as they seem to provide the appropriate Brønsted/Lewis balance[3]. Among all the existing morphologies in the silica-based family, the newly developed dendritic silica particles are particularly promising. They indeed offer a unique radial pore system that is expected to promote an improved diffusion of reactants and products throughout the material[4]. Dendritic materials remain however largely underexplored in the context of CO_2 conversion. In this work, this particular morphology was therefore exploited in combination with the insertion of hafnium atoms into the structure and the grafting of imidazolium groups. These modifications provided an efficient heterogeneous bifunctional catalyst displaying improved catalytic performances compared to the monofunctional counterpart, while also demonstrating recyclability over consecutives catalytic cycles.



Objectives of the project.



Recycling of the catalyst over consecutive cycles for the conversion of styrene oxide and CO_2 (25 bar, 125°C, 3h).

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Community detection via matrix factorization under the degree-corrected block model

Alexandra Dache, Arnaud Vandaele and Nicolas Gillis
Department of Mathematics and Operationnal Research, University of Mons
alexandra.dache@umons.ac.be

Community detection is a fundamental task in data analysis, helping us to understand how the elements of a network organize and interact. Block models provide an approach for identifying a wide variety of community structures while offering high interpretability. The degree-corrected block model (DCBM) [1] is particularly useful as it accounts for variation in node connectivity within communities. However, standard inference methods for the DCBM are computationally costly and highly sensitive to initialization, while cheaper alternatives such as spectral or modularity-based approaches are limited to detecting specific structures. In this work, we show that the inference of the DCBM can be reformulated as a constrained nonnegative matrix factorization problem. Leveraging this insight, we propose a novel method for community detection and a theoretically well-grounded initialization strategy that provides an initial estimate of communities for inference algorithms. Our approach improves both efficiency and accuracy in identifying communities. For further details, see [2].

References

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Study of The Inhibition of LDH by Covalent SuFEx Inhibitors

Julie Dullier[1], *Mégane Van Gysel*[1], *Xavier Garcia Llinàs*[2], *Lionel Pochet*[2] & *Johan Wouters*[1]
[1]Laboratory of structural and biological chemistry (CBS) - Namur Research Institute for Life Sciences (Narilis), Department of Chemistry, University of Namur
[2]Namur Research Institute for Life Sciences (Narilis), Departement of Pharmacy, University of Namur
julie.dullier@unamur.be

Lactate dehydrogenase (LDH) is a promising target for cancer therapy, given its role in supporting tumor growth. LDH catalyzes the interconversion of pyruvate to L-lactate in the presence of the NAD cofactor at the end of the glycolytic pathway.(1) Because targeting the active site of LDH suffers from several drawbacks,(1,2,3) this research explores an approach targeting LDH's tetramerization interface.

Collaborators of UCLouvain have identified two allosteric sites, as potential targets for disrupting LDH tetramer assembly.(4) Fluoxetine and sertraline have been identified as modulators that target these sites.(5) To enhance their inhibitory potency, the aim of this work is to synthesize targeted covalent inhibitors (TCIs) using a sulfonyl fluoride warhead (-SO_2F) used thanks to the Sulfur(VI) Fluoride Exchange (SuFEx) reaction.(6) An illustration of the principle is presented in Figure 1.

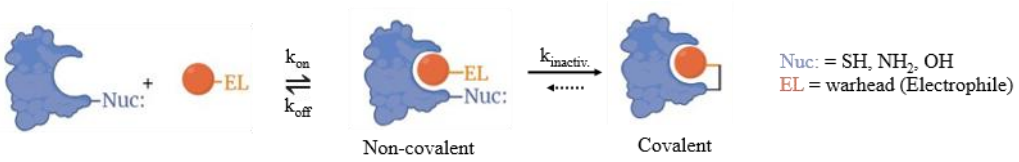

Figure 1: Scheme of the mode of action of covalent inhibitor (Figure adapted from Bauer RA. and al.(7) and Lagoutte R and al.(8))

Our results demonstrate the successful synthesis of modified fluoxetine and sertraline derivatives. Covalent docking studies have revealed the binding mode of these TCIs to LDH, and enzymatic assays allowed determination of the inhibitory activity of the ligands against LDH-B. Our findings suggest that targeting LDH's tetramerization interface with TCIs is a promising novel strategy for cancer treatment

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Avalanche size distributions in sandpile model on complex networks

Komlan Fiagbe
Naxys, Department of Mathematics, University of Namur
komlan.fiagbe@unamur.be

Avalanche dynamics in driven threshold systems can display intermittent bursts of activity spanning a broad range of sizes. In this seminar, I will focus on (BTW) sandpile model implemented on complex network topologies, such as scale-free graphs, random regular graphs... Using numerical simulations together with analytical approximations, I will examine how local toppling rules generate avalanche patterns, how avalanche size distributions emerge, and how their scaling properties are shaped by network structure. Particular attention will be paid to distinguishing genuine power law and to identifying which structural and model parameters control these regimes.

Keywords: Sandpile model, Network, Powerlaw

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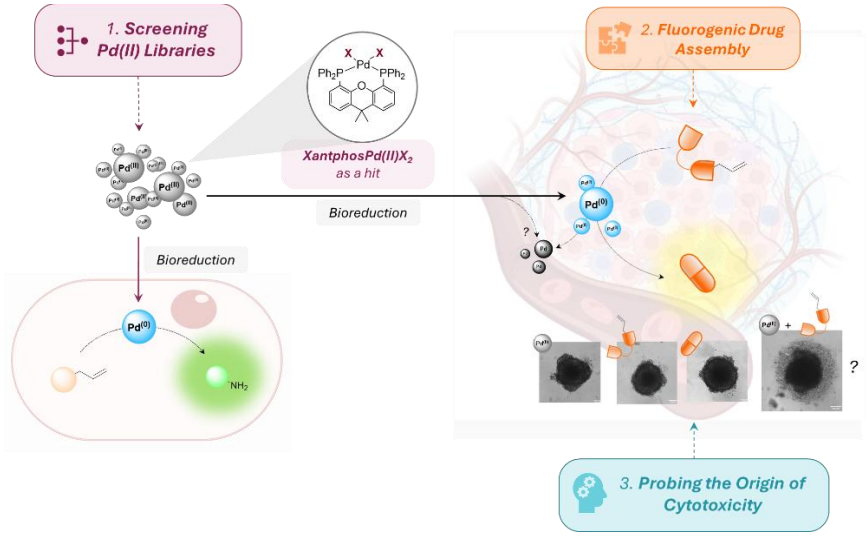
Bioorthogonal Pd-Catalyzed Anticancer Prodrug Activation: *When Chemistry Drives Cytotoxicity*

LEFÈVRE Marine [a, b], *FERON Olivier* [b], *RIANT Olivier* [a]
[a]Institute of Condensed Matter and Nanosciences, MOST, UCLouvain
[b]Institute of Experimental and Clinical Research, FATH, UCLouvain
marine.lefevre@uclouvain.be

Cancer cells are often described as chemically "rewired": altered metabolism and redox balance can create a more reducing intracellular environment. For bioorthogonal palladium catalysis, this is both an opportunity and a risk—Pd(II) precatalysts may be activated where we want them, but the same chemistry can also generate unanticipated species that dominate biological outcomes.

Here we explored a Pd-mediated drug-assembly strategy in cells, built on the premise that intracellular reduction can convert Pd(II) complexes into catalytically competent Pd(0) for prodrug activation. An *in cellulo* catalyst screen identified Xantphos-type Pd(II) scaffolds as particularly promising, consistent with efficient bioreduction and robust uncaging reactivity under cellular conditions. However, when translated to a therapeutic aminocoumarin platform, a discrepancy emerged: viability assays revealed pronounced cytotoxicity that did not match the expected behavior of the assembled drug.



This shifted the central question from "Does the prodrug generate the intended product?" to "What chemistry actually occurs in cells?" By combining time-resolved $^{1}H/^{31}P$ NMR with LC–MS/HPLC profiling, we tracked palladium speciation alongside product evolution under cell-relevant conditions. These analyses revealed formation of an unanticipated reaction product (and associated Pd species) whose emergence correlates with loss of viability, indicating that the dominant cytotoxic agent can arise from the Pd-mediated transformation rather than from the designed payload alone. Overall, this work highlights palladium speciation as a controlling variable in bioorthogonal anticancer prodrug activation and underscores the need to pair in cellulo reactivity readouts with product/speciation analysis to correctly assign the origin of cytotoxicity.

Shine Bright Like a Diamond - Even Under Stress: Modeling Spectral Shifts of Strained Color Centers

E. Aylin Melan[1,2,3], *Danny E. P. Vanpoucke*[2,3], *Luc Henrard*[1]
[1] NISM and Physics department, University of Namur
[2] QuATOMs, Materials Chemistry, Hasselt University
[3] imo-imomec, imec vzw, Hasselt University
EsinAylin.Melan@UHasselt.be

Diamonds are not only a girl's best friend, but also of many scientists. Outside of the scientific community, it is known as a pretty gemstone that comes in different shapes and colors, ideal for sparkly jewelry. However, behind that sparkle, diamonds can have imperfections. Imperfections that can give the gemstone interesting colors, associated with crystallographic defects called color centers.[1] These give diamond suitable properties for a variety of high-end quantum applications as quantum bits. One such color center is the Germanium-vacancy (GeV). It is a highly symmetric (D_{3d}) defect center resulting in a sharp spectral peak, the zero-phonon line (ZPL), making it a promising candidate for a single photon emitter needed for quantum communication applications.

Strains, however, have an impact on the spectral properties of color centers. It can break the symmetry and alter the optical properties.[2] In this work, density functional theory is used to model the ZPL of the GeV under hydrostatic and linear strain. Hydrostatic strain does not break the symmetry of the defect. There is, however, a difference in spectral shift under tensile and compressive strain. It has a red- and blue-shift, respectively. Linear strain does break the symmetry and results in C_{2h} symmetry. The breaking of symmetry, due to both tensile and compressive strain, results in a red-shift of the ZPL. Additionally, the GeV center can be in different charge states and can be influenced differently by strain. Therefore, further theoretical studies are needed to understand the observed optical properties.

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Toward Greener Lithium-Ion Batteries: Water-Based Processing of NMC Cathodes

Driélle Müller[a,b,c,], Cédric Vandenabeele[a,b], Nathalie Job[c], Stéphane Lucas[a,b]*

[a] *Laboratoire d'Analyse par Réaction Nucléaires (LARN), Namur Institute of Structured Matter (NISM), University of Namur, 61 Rue de Bruxelles, 5000 Namur, Belgium*
[b] *Innovative Coating Solutions (ICS), 10, Rue Jean Sonet, B-5032 Isnes, Belgium*
[c] *Department of Chemical Engineering – Nanomaterials, Catalysis, Electrochemistry (NCE) University of Liège (B6a), 4000 Liège, Belgium*

E-mail: drielle.mullerdasilva@unamur.be

The transition toward more sustainable lithium-ion battery manufacturing requires replacing toxic organic solvents used in electrode fabrication with environmentally benign alternatives such as water. While aqueous processing is already well established for anodes, its application to nickel-rich cathode materials remains challenging due to their high reactivity with water, which leads to surface degradation, lithium leaching, and performance loss [1,2]. This PhD project investigates the physicochemical mechanisms governing the interaction between layered NMC cathode materials and water during electrode processing, with a focus on NMC532. Particular attention is given to the role of slurry composition, binder chemistry, and pH evolution in controlling lithium stability and electrode performance. Systematic pH measurements reveal that aqueous processing induces alkalinization through surface-limited and equilibrium-limited lithium leaching mechanisms, whose relative contributions depend strongly on material concentration and chemical environment. The influence of different binders is examined, highlighting that xanthan gum-based formulations moderate pH evolution differently from conventional water-soluble binders such as CMC, suggesting a binder-dependent control of lithium leaching pathways. Electrochemical testing shows that while optimized aqueous processing can achieve performance comparable to conventional PVDF/NMP routes for NMC532, the same strategies are not directly transferable to more reactive NMC811 materials. Overall, this work provides mechanistic insight into water-based cathode processing and outlines pathways toward greener lithium-ion battery manufacturing compatible with high-energy cathode materials.

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From Invasive Plants to Disease Risk: An Overlooked One Health Perspective

Tasneem Osman
Laboratory, Department, University
Tasneemmoawia@uni-bonn.de

Sustainable and healthy communities rely on a safe environment in which ecological change does not exacerbate disease risk for humans, livestock and wildlife.
Mosquito-borne diseases, including zoonotic arboviruses, are strongly influenced by environmental conditions that affect mosquito survival, abundance, and dispersal. However, disease control strategies have largely emphasized human-mosquito interactions and aquatic larval habitats, breeding sites, while the role of vegetation in mosquito ecology and transmission dynamics remains underexplored.
Plants play a substantial role in mosquito life cycles by providing essential sugar supplies and influencing microclimatic conditions that affect survival, resting behaviour, and population persistence. Despite this, the role of vegetation in mosquito ecology has been largely neglected as vector control tactics. The spread of invasive alien plant species is particularly relevant because these plants frequently expand rapidly, disrupt ecosystem structure, and create favourable conditions for mosquitoes. Increased dominance of invasive plants could sustain high mosquito populations and favor competent mosquito species, raising the risk of malaria and arboviral transmission, such as dengue, Zika, chikungunya, and West Nile virus.
Vegetation, particularly invasive plant species, represents a critical yet frequently overlooked component of mosquito ecology. Integrating invasive plant management into malaria and arboviral control strategies offers a sustainable approach to strengthening public health protection while supporting ecosystem balance. Achieving long-term, sustainable reductions in the burden of mosquito-borne diseases will require interdisciplinary approaches that integrate ecology, climate science, and public health. Vegetation, especially invasive plant species, constitutes a vital although often neglected aspect of mosquito ecology. Integrating invasive plant management into malaria and arboviral control techniques provides a sustainable method for enhancing public health protection and maintaining environmental equilibrium. Attaining enduring, sustainable decreases in the prevalence of mosquito-borne diseases necessitates interdisciplinary strategies that integrate ecology, climate science, and public health.

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Multimodal Imaging Biomarkers of Lesion Severity and Functional Outcome in a Rat Model of Cervical Spinal Cord Injury

Claudia Schrauwen[1,2,3], *Ignace Van Spilbeeck*[1,2], *Johan Van Audekerke*[1,2], *Annemie Van Eetveldt*[4], *Nicolas Halloin*[3], *Zoë Laermans*[1], *Winnok H. De Vos*[2,5,6], *Aleksandar Jankovski*[7], *Marleen Verhoye*[1,2], *Charles Nicaise*[3], *Daniele Bertoglio*[1,2]

1Bio-Imaging Lab, University of Antwerp, Antwerp, Belgium
2μNeuro Center for Excellence, University of Antwerp, Antwerp, Belgium
3URPhyM–NARILIS, University of Namur, Namur, Belgium
4Molecular Imaging Center Antwerp, University of Antwerp, Antwerp, Belgium
5Laboratory of Cell Biology and Histology, University of Antwerp, Antwerp, Belgium
6Antwerp Centre for Advanced Microscopy, University of Antwerp, Antwerp, Belgium.
7Departement of Neurosurgery, Vivalia Hospital, Arlon, Belgium

Presenting author: claudia.schrauwen@uantwerpen.be

Traumatic spinal cord injury (SCI) causes persistent motor and sensory deficits and remains a major cause of disability, with cervical injuries accounting for nearly half of all cases[1,2]. Despite promising preclinical therapies, clinical translation is limited by the lack of non-invasive biomarkers that reliably reflect injury severity and tissue integrity. This study aimed to establish quantitative magnetic resonance imaging (MRI) and positron emission tomography (PET) markers of lesion pathology following graded cervical contusion SCI in rats.

Nine-week-old female rats received a unilateral C5 contusion[3] (100, 250, or 400 kDyn; n=10/group) or sham laminectomy (n=10). Forelimb motor function was assessed for up to 6 weeks post-injury using the Irvine Beatties Bresnahan (IBB) test[4]. Longitudinal *in vivo* imaging included structural MRI, T2 mapping, and diffusion MRI to quantify lesion volume and microstructural changes, alongside [^{18}F]SynVesT-1 PET/CT targeting synaptic vesicle glycoprotein 2A (SV2A) at 1 and 6 weeks post-SCI.

Functional recovery depended on injury severity, with severe injuries showing delayed improvement. MRI revealed that lesion volumes decreased over time but persistent differences between lower and higher severity groups indicated lasting effects of the initial trauma. Diffusion and T2 metrics captured complementary aspects of axonal degeneration and demyelination. [^{18}F]SynVesT-1 PET demonstrated significant and persistent SV2A loss at the injury site compared to shams, with greater reductions in severe injuries and no recovery by 6 weeks.

Together, these findings show that combined MRI and SV2A PET provide sensitive, translatable biomarkers of graded SCI pathology and recovery, supporting their use in therapeutic evaluation.

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The Joint Effect of Stressor Diversity and Biodiversity on Ecosystem Function in Algal Communities

Laura Willam
Research unit in environmental and evolutionary biology (URBE), Biology,
University of Namur
lauralns@outlook.be

My project aims to understand the effects of complex mixtures of environmental stressors on ecosystems. Biodiversity mitigates these effects, but this protection may diminish as stressors increase [1, 2, 3]. This work will be the first to examine the joint effect of biodiversity and stressor diversity (the number of stressors, stressor richness, and their similarities) on ecosystem function [4, 5], using algal communities as a model. In WP1, I will assess the responses of 10 algal species to 9 stressors and their combinations. I will quantify how stressor diversity affects response diversity and hypothesize that stressor richness positively affects response diversity, whereas stressor similarity increases response diversity [4, 5]. In WP2, I will conduct an experiment combining biodiversity and stressor diversity treatments to measure ecosystem function. I hypothesize that biodiversity will protect the ecosystem less when stressor diversity is high and similar. I will also investigate how species-level stressor interactions affect my results. WP3 will use mathematical modelling to test whether these effects can be predicted using data from my project and the literature. This research will advance ecology and conservation by refining ecological predictions in the face of global change.

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Can You Be More Explicit? A Task and Dataset on Explicitations of Implicit Meaning

Laura Zeidler
Technical University of Nuremberg

Making texts clear and comprehensible has become an increasingly important topic in NLP. With the long-term aim of facilitating enhanced comprehension of instructional texts by making implicit meaning explicit, we study cases of so-called explicitations, i.e.~revisions that render implicitly conveyed content explicit. Using revision histories from wikiHow, we propose a rule-based approach to automatically extract candidate explicitations and we curate an annotated dataset in which explicitations are distinguished from insertions of new information.

Our analyses show that while the extraction method is effective in retrieving relevant cases, distinguishing explicitations from new information is a challenging and often subjective task, reflecting differences in background knowledge and reasoning. Experimentally, we find some LLMs to achieve competitive performance in zero-shot settings, but gains from few-shot prompting and fine-tuning are inconsistent. In contrast, fine-tuned NLI models benefit consistently from supervised training and show stronger robustness under distribution shift. Overall, our findings highlight the subjective nature of explicitations and the difficulty of reliably distinguishing them from insertions of new information, while also showing that the annotated data contains informative signals that models can learn from.

Posters Abstracts

The third scaling law, no one talks about

Marthe Ballon

Large language models have demonstrated remarkable progress in mathematical reasoning, leveraging chain-of-thought and test-time compute scaling. However, many open questions remain regarding the interplay between reasoning token usage and accuracy gains. In particular, when comparing models across generations, it is unclear whether improved performance results from longer reasoning chains or more efficient reasoning. We systematically analyze chain-of-thought length across o1-mini and o3-mini variants on the Omni-MATH benchmark, finding that o3-mini (m) achieves superior accuracy without requiring longer reasoning chains than o1-mini. Moreover, we show that accuracy generally declines as reasoning chains grow across all models and compute settings, even when controlling for difficulty of the questions. This accuracy drop is significantly smaller in more proficient models, suggesting that new generations of reasoning models use test-time compute more effectively. Finally, we highlight that while o3-mini (h) achieves a marginal accuracy gain over o3-mini (m), it does so by allocating substantially more reasoning tokens across all problems, even the ones that o3-mini (m) can already solve. These findings provide new insights into the relationship between model capability and reasoning length, with implications for efficiency, scaling, and evaluation methodologies.

Insight into the processing mechanism of secreted bacterial intein-like domains

Marion Bauwens
BGM, LIBST, UCLouvain
marion.bauwens@uclouvain.be

Bacterial intein-like domains (BILs) belong to the Hint (Hog/INTein) superfamily, which also includes inteins and Hog domains. Hints are auto-proteolytic domains that are inserted into host proteins and can catalyze their own splicing while ligating the flanking sequences. In this project, we investigated the autocatalytic mechanism of extracellular bacterial intein-like domains that are naturally embedded in large extracellular proteins from the plant pathogen *Pseudomonas*. Interestingly, we discovered that, upon excision, these BILs catalyze a peptide hydrolysis reaction by connecting the two flanking polypeptides end up via a disulfide bridge. We also demonstrated the possibility of controlling the peptide cleavage through disulfide reduction. Overall, these BIL domains act as maturation domains that could be used in biotechnology or synthetic biology, for instance in the design of autocleavable linkers or modules for conditional protein inactivation.

Association of frailty and sarcopenia with amyloid positivity

Emma Calluy[1,2], Médea Locquet[3], Jean-Yves Reginster[4], Olivier Bruyère[5], Etienne Cavalier[2], Aurélie Ladang[2], Charlotte Beaudart[1]

[1]Public Health Aging Research & Epidemiology (PHARE) Group, Research Unit in Clinical Pharmacology and Toxicology (URPC), NAmur Research Institute for LIfe Sciences (NARILIS), Faculty of Medicine-Department of biomedical Sciences, University of Namur, 61, Rue de Bruxelles, 5000 Namur, Belgium.

[2]Department of Clinical Chemistry, Center for Interdisciplinary Research on Medicines, Centre Hospitalier Universitaire de Liège, University of Liège, Avenue de l'Hôpital 1, 4000 Liège, Belgium., Liège, Belgium.

[3]Research Unit in Clinical Pharmacology and Toxicology (URPC), NAmur Research Institute for LIfe Sciences (NARILIS), Faculty of Medicine-Department of pharmacy, University of Namur, 61, Rue de Bruxelles, 5000 Namur, Belgium.

[4]Protein Research Chair, Biochemistry Department, College of Science, King Saud University, Riyadh, Kingdom of Saudi Arabia., Riyadh, Saudi Arabia

[5]Research Unit in Public Health, Epidemiology and Health Economics, University of Liège, Liège, Belgium.

emma.calluy@unamur.be

Objective: The statistical association between multidimensional geriatric syndromes and amyloid positivity is not currently well understood. Yet, a better understanding of this clinical association could enable general practitioners to use easy-to-use tools to help with screening for cognitive decline. Using the Sarcopenia and Physical Impairment with advancing Age (SarcoPhAge) study, a Belgian cohort study including older adults, this study aims to evaluate if an association between the blood concentration of phosphorylated tau at position 217 (pTau217), a biomarker of amyloid positivity, and components of sarcopenia and frailty may exist.

Material and Methods: The concentration of pTau217 was measured in 218 plasma samples on Lumipulse platform at the second year of follow-up of the cohort. pTau217 was categorised according to recent literature in pTau 217 <0.13 pg/mL= amyloid-negative, pTau217= 0.13-0.39 pg/mL= possibly amyloid-positive, pTau217 >0.39 pg/mL= amyloid-positive. Sarcopenia and frailty components were evaluated and categorised according to the European Working Group on Sarcopenia in Older People (EWGSOP2) and Fried criteria, respectively.

Results: The 218 participants from the SarcoPhAge study had a median age of 73.96 years (interquartile range (IQR)= 69.57-78.49), 51% were women and the median concentration of pTau217 was 0.09 pg/mL (IQR=0.06-0.18). Based on predefined cut-offs, 140 participants were classified as amyloid-negative, 65 as possibly amyloid-positive, and 13 as amyloid-positive. Regarding geriatric status, 13 participants were sarcopenic, 9 were severely sarcopenic, 17 were frail, and 97 were pre-frail.

When all variables were analysed continuously, no significant correlations between pTau217 and handgrip strength, short physical performance battery (SPPB), gait speed, chair stand speed, appendicular lean mass and lean mass were found (p>0.05). When categorised, sarcopenia and frailty, low gait speed, low SPPB, low muscle strength and low muscle mass in women were not significantly associated with pTau217 concentration (p>0.05). Additionally,

the number of participants with amyloid positivity was not significantly higher in participants diagnosed with sarcopenia or frailty nor with participants with lower gait speed, lower SPPB, lower muscle mass or lower muscle strength ($p>0.05$).

Nonetheless, in addition to a significant association of pTau217 with Body Mass Index (BMI) ($p=0.02$), this study demonstrated a significantly correlation of pTau217 with fat mass ($p<0.01$). Moreover, low muscle mass was associated with higher concentrations of pTau217, but exclusively in men ($p=0.006$).

Conclusion(s): The clinical components of frailty and sarcopenia did not demonstrate an association with pTau217 in this study, suggesting that geriatric syndromes are not associated with cognitive decline. Nevertheless, it would be worthwhile investigating this association in a longitudinal study involving clinical evaluations of cognitive decline.

Drugging the Endoplasmic Reticulum Exit Sites

Lucie Caramelle[1], Antonella Capuozzo[2], Mégane Van Gysel[3], Diego Medina[2], Johan Wouters[3], Alison Forrester[1,4]

[1]Research Unit of Biochemistry and Cell Biology (URBC), Namur Research Institute for Life Sciences (NARILIS), University of Namur, Belgium

[2]Telethon Institute of Genetics and Medicine (TIGEM), Pozzuoli, Italy

[3]Department of Chemistry, NAmur MEdicine & Drug Innovation Center (NAMEDIC-NARILIS), University of Namur, Belgium

[4]WEL Research Institute, Avenue Pasteur, 6, 1300 Wavre, Belgium

lucie.caramelle@unamur.be

The biosynthetic pathway is comprised of multiple steps during which nascent proteins undergo modification and folding. Beginning in the Endoplasmic Reticulum (ER), proteins are then transported to the Golgi for post-translational modification and finally distributed throughout the cell or secreted. Aberrant secretion of proteins can cause a wide range of diseases. One of the most common being fibrosis, where the excessive production and accumulation of extracellular matrix components leads to a loss of function of tissues and organs. In 2019, fibrotic disease was implicated in > 35% of deaths worldwide[1]. Despite this, no effective treatment currently exist.

Small molecule Retro-2 has been discovered as an inhibitor of retrograde transport that targets ER exit site (ERES) protein Sec16A, slowing anterograde trafficking of SNARE protein Syntaxin5[2,3]. Retro-2 thus illustrates that targeting ERES proteins can modulate anterograde trafficking. We have investigated other compounds to study molecular factors influencing the secretory pathway and their roles in cellular processes.

Using a microscopy-based readout of anterograde trafficking of 5 cargo proteins (type I pro-collagen, RUSH Mannosidase II, TNFα, GPI-anchored proteins and ssGFP[4]), we screen compounds for their modulatory effects on ER-Golgi trafficking, in a 3-tiered approach: i) testing chemically diverse compounds, ii) testing structurally similar compounds to hits identified in (i), iii) building the pharmacophore of hits to computationally screen wider libraries, before testing them experimentally. Additionally, compounds were excluded using the cell painting assay[5] to analyse the effects of compounds on global cellular pathways. Cellular thermal shift assays (CETSA) have identified Sec16A as the target of hit Compound Y, and other hits are currently being analysed. Mass spectrometry and procollagen trafficking assays show that compound Y slows the trafficking and secretion of type I collagen. Compound Y will now be tested in models of fibrosis, while CETSA will be used to identify the target proteins of other hit compounds in the pathway.

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ERES, GATOR2 and NPC: Is complex activity determined by Sec13?

Ines de Fays[1], Lucie Caramelle[1], Utku Horzum[2] Alison Forrester[1,3]
[1] Research Unit of Cell Biology (URBC), Namur Research Institute for Life Sciences (NARILIS), University of Namur, Rue de Bruxelles 61, 5000 Namur, Belgium
[2] Institute of Pathophysiology, Medical University of Innsbruck, Innsbruck, Austria
[3] WEL Research Institute, Avenue Pasteur, 6, 1300 Wavre, Belgium
ines.defays@unamur.be

Endoplasmic Reticulum Exit Sites (ERES) are sites of COPII carrier formation deputed to trafficking nascent proteins from ER to Golgi. Proper regulation is crucial for cellular homeostasis, and dysregulation is associated with various diseases. Sec13 is a member of the ERES complex, binding to "scaffold" protein Sec16A as well as outer coat protein Sec31. Sec13 is also a member of mTORC1 regulatory complex GATOR2, and the Nuclear Pore Complex (NPC). All three complexes regulate pathways that require high levels of ATP, which leads to the question, are these processes active at the same time, or is their activation regulated to balance the anabolic load of the cell?

Compound X is a novel and specific inhibitor of ERES. It targets Sec16A and causes a dissociation from Sec13, slowing ER to Golgi trafficking of Pro-collagen type II. An optimised version, Compound X-OPT has the same effects, with amplified efficacy. We hypothesise that decreasing the interaction between Sec16A and Sec13 may release Sec13 to interact more with mTORC1 and/or NPC, balancing anabolic processes.

Using Compound X as a tool to decrease Sec13 binding to Sec16, this project characterises the impact of an increased pool of "free" Sec13 on cellular homeostasis. Co-immunoprecipitation of SNAP-Sec13 in CRISPR/Cas9 knock-in HeLa cells shows that Compound X decreases interactions between Sec13 and partners Sec16A (15%), WDR59 (23%) and Nup96 (12%) while Compound X-OPT causes an amplified loss of interaction: Sec16A (18%), WDR59 (36%) and Nup96 (38%). Interestingly, the Sec13-Sec31A interaction is maintained. Degradation of the proteins was not induced by compound treatment.

Next, we will study the functional effects of Compounds X and X-OPT on non-ERES processes GATOR2 and NPC. Using Western blots we will measure mTORC1 activation. Preliminary data shows that Compound X-OPT decreases proliferation in professional secretory cells. We will confirm this using FACS to study cell cycle, a GFP-NLS/NES-based assay to measure nucleocytoplasmic shuttling, and immunofluorescence to count the number of NPC per cell. This data will describe the effect of free Sec13 on cellular homeostasis, and form the foundation as to whether Sec13 balances anabolic processes physiologically.

Embryos at risk: Early embryonic development of aquatic ectotherms in a warming and polluted world

Nicole GOEDE [1,2,3], Eli THORÉ [3,4,5], Luc BRENDONCK [2,6], Lendert GELENS [1]

1 Laboratory of Dynamics in Biological System, Department of Cellular and Molecular Medicine, KU Leuven, Belgium
2 Laboratory of Animal Ecology, Global Change and Sustainable Development, Department of Biology, KU Leuven, Belgium
3 Laboratory of Adaptive Biodynamics, Research Unit in Environmental and Evolutionary Biology (Department of Biology), Institute of Life, Earth, and Environment, University of Namur, Belgium
4 Department of Wildlife, Fish, and Environmental Studies, Swedish University of Agricultural Sciences, Sweden.
5 TRANSfarm, Science, Engineering, and Technology Group, KU Leuven, Bijzondereweg 12, 3360 Bierbeek, Belgium.
6 Water Research Group, Unit for Environmental Sciences and Management, North-West University, South Africa

nicole.goede@kuleuven.be

Animals increasingly face harsh environmental conditions, including exposure to rising temperatures and chemical pollutants. Egg-laying ectotherms—including many fishes and amphibians—may be particularly vulnerable to a changing environment during early embryonic stages. Yet, the effects of temperature and chemical exposure on their early embryonic development have received little attention and remain poorly understood. Predicting these effects is further complicated by the fact that simultaneous exposure to rising temperatures and pollutants—a common situation in natural settings—can result in complex interactive effects beyond the sum of their individual impacts.

To address this knowledge gap, we use advanced imaging techniques to capture high-resolution spatiotemporal data on embryonic development in three model species: *Xenopus laevis, Danio rerio,* and *Nothobranchius furzeri*. We quantify the temperature-dependent scaling of key developmental events within each species and assess how these patterns interact with chemical exposure.

Ultimately, this research will advance our understanding of the fundamental principles that regulate early life. Thereby, these insights will allow for more accurate predictions of how aquatic animals respond to global change, particularly under combined temperature and chemical stress.

Towards reconstituting meiotic crossover formation

Veronica Gonzalez, Corentin Claeys Bouuaert
Louvain Institute of Biomolecular Science and Technology, Université catholique de Louvain
veronica.gonzalez@uclouvain.be

During meiosis, the paternal and maternal homologous chromosomes exchange DNA fragments by crossing over, which arises by a complex and tightly regulated DNA recombination pathway initiated by the programmed induction of DNA double-strand breaks. Breaks are resected to leave 3' single stranded tails that invade a homologous template to initiate repair. A subset of recombination intermediates are stabilized by a family of proteins called ZMM that include MutSγ (Msh4-Msh5), the ZZS complex (Zip4, Zip2, Spo16), Zip3 and Mer3. Recombination intermediates stabilized by ZMM proteins mature into double Holliday Junctions (dHJ), which are resolved specifically as crossovers by MutLγ together with Exo1, dependent on the Cdc5 kinase. However, how these proteins collaborate to drive crossing over remains unclear. We will present our biochemical approach aimed at investigating the molecular mechanism of crossing over *in vitro*.

Towards a core outcome set for sarcopenia intervention studies: results from a delphi study

Van Heden S[1]., Sanchez-Rodriguez D[2-3]., Bruyère O[4]., Reginster J-Y[5]., Surquin M[2]., Beaudart C[1].

1 Public Health Aging Research & Epidemiology (PHARE) Group, Research Unit in Clinical Pharmacology and Toxicology (URPC), Department of Biomedical Sciences, Namur Research Institute for Life Sciences (NARILIS), Faculty of Medicine, University of Namur, 5000 Namur, Belgium

2 Geriatrics Department, Brugmann University Hospital, Université Libre de Bruxelles, 1020 Brussels, Belgium

3 Rehabilitation Research Group, Hospital del Mar Research Institute, 08003 Barcelona, Spain

4 Research Unit in Public Health, Epidemiology and Health Economics, Department Physical Activity and Rehabilitation Sciences, University of Liège, Liège, Belgium

5 Protein Research Chair, Biochemistry Department, College of Science, King Saud University, Riyadh, Kingdom of Saudi Arabia

Email of presenting author: sophievanheden@unamur.be

Background: A Core Outcome Set (COS) specific to sarcopenia is currently being developed to address the significant heterogeneity observed in outcome assessment in clinical trials. A COS is defined as "*an agreed standardized set of outcomes that should be measured and reported, as a minimum, in all clinical trials in specific areas of health or health care*". The development process involves several steps: a scoping review identifying 253 outcomes, patient interviews leading to 3 additional outcomes, the present Delphi study, and a final consensus process conducted by a multidisciplinary working group. Therefore, this study aims to establish expert consensus on the most relevant outcomes to inform the development of a COS for sarcopenia clinical trials.

Methods: A two-round Delphi study including international experts in sarcopenia evaluated 34 outcomes derived from the scoping review and patient interviews. Experts rated the importance of each outcome for inclusion in a common COS applicable to all intervention types and in intervention-specific sub-COSs (exercise, nutrition, and pharmacological) using a 9-point Likert scale (1 = not important; 9 = critically important). Consensus was defined as ≥75% of ratings between 7–9 ("consensus in") or ≥15% between 1–3 ("consensus out"). Expert voting was supported by Welphi software, and descriptive analyses were performed using RStudio.

Results: A total of 133 (round I) and 80 experts (round II) completed the survey. After completion of both rounds, 16 outcomes reached consensus for inclusion in the common COS. These outcomes, listed in descending order of consensus (≥75%), included muscle strength, falls, sarcopenia status, physical performance, mortality, physical status, activities of daily living, quality of life, frailty status, nutritional status, muscle mass, need for assistance, institutionalization, hospitalization, adverse events, and muscle power.

Additional outcomes reached consensus only within intervention-specific sub-COSs. For example, appetite reached consensus for nutrition-based interventions, while cardiopulmonary function reached consensus for exercise-based interventions.

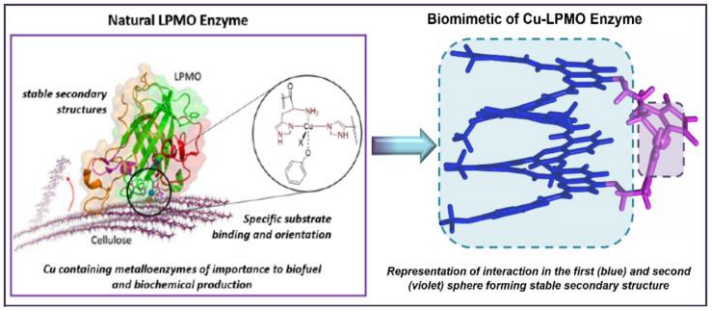
Conclusion: The selected outcomes will inform the final stage of the COS development process, including a multidisciplinary consensus meeting to formally agree on the final Core Outcome Set for sarcopenia clinical trials.

Development of Multi-Layered Biomimetic Scaffold for Lytic Polysaccharide Monooxygenases (LPMOs) Using the Histidine Brace

*Saima Kamaal, Michael Singleton**
Institute of Condensed Matter and Nanosciences (IMCN),
Laboratoire de chimie supramoléculaire et biomimétique,
Université Catholique de Louvain, Place de l'Université 1, 1348 Louvain-La-Neuve, Belgium
Email : saima.kamaal@uclouvain.be

Lytic polysaccharide monooxygenases (LPMOs) have revolutionized the enzymatic processing of polysaccharides, especially recalcitrant insoluble polysaccharides like cellulose[1]. These are a family of copper containing metalloenzymes important for biofuel and biochemical production due to their ability to oxidatively cleave the strong glycosidic C-H bonds in cellulose. The active site of LPMO consists of a single Cu atom bound in a T-shaped N3 coordination environment consisting of an N-terminal histidine imidazole and NH_2 and a second histidine imidazole trans to the first, this motif is called the histidine brace[2]. The same structure is also found in particulate methane monooxygenase suggesting that the histidine brace is responsible for the oxidative capabilities of the enzymes[3]. However, the specific role of histidine brace as well as many other structural features of the active site are still unclear.

The systematic study of metal complexes containing specific structural modifications, can facilitate the isolation and understanding of how these changes affects complex's behaviour. Herein this poster we aim to discuss strategy to develop more accurate active site mimics for LPMOs through multi-layered coordination scaffold using foldamers with a focus on understanding the importance of the different structural features of the histidine brace motif for oxidative reactivity. Through systematic variation of both first and second coordination spheres, we aim to define the important features necessary in biomimetic copper complexes for the oxidation of C-H bonds with high bond dissociation energies. Ultimately, this work will contribute to the design of more efficient and robust catalysts for industrial applications.



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Crystallisation and structural studies of 4-aminopyridine (4-AP) salt derivatives and 1-H imidazolium chloride

***A. Kundu*[1], *L. Fusaro*[2], *N. Tumanov*[3], *K. Bucar*[3], *R. Montis*[4]**

[1] Laboratory of Applied Materials Chemistry, UCNANO, Department of Chemistry, Namur Institute of Structured Matter (NISM), University of Namur, Belgium

[2]Technological platform for physicochemical characterization (PC[2]), Namur Institute of Structured Matter(NISM), University of Namur, Belgium

[3]Department of Chemistry, University College London, United Kingdom

[4]Department of Pure and Applied Sciences – DISPeA, University of Urbino, Italy

Email: anita.kundu@unamur.be

Crystallisation is the key separation and purification process in the pharmaceutical and fine chemical industries, where control over crystal size, morphology, and solid form is essential for product quality and downstream processing.[1] However, during crystallisation development, liquid–liquid phase separation (LLPS), often referred to as oiling out, has emerged as a widely observed phenomenon.[2] During LLPS the solution undergoes supersaturation, forming a dense liquid phase and promoting nucleation and crystallisation by reducing solute solubility.[3-5]

We previously studied the crystallisation of 4-aminopyridinium chloride (4AP-HCl) from aqueous solutions. In the presence of acetone, it undergoes an LLPS, followed by the crystallisation of complex structures belonging to the Frank–Kasper (FK) phases, a particular family of topologically close-packed structures that have never been observed in small and rigid molecules [3,4]

The aim of this work is to understand the role of LLPS in the crystallisation of complex phases of other simple salts. Here, we describe our investigations on a family of 4-aminopyridinium salts, such as 4-aminopyridinium bromide(4AP-HBr), 4-amino-2-fluoropyridinium chloride(2F-4AP-HCl), 4-amino-3-fluoropyridinium chloride(3F-4AP-HCl), and 1H-imidazolium chloride (IMI-HCl). Crystals of the target compounds were obtained from a dense liquid phase and separated in the presence of acetone. The resulting crystals were then characterised by single-crystal X-ray diffraction (SCXRD).

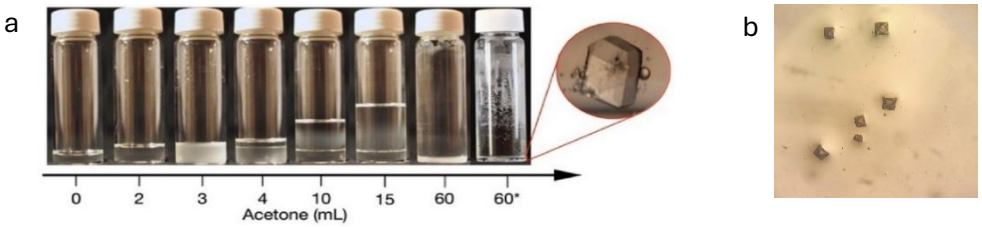

Figure 1: a) Antisolvent LLPS crystallization of 4AP-HCl.[5] b) Single crystals of 2F-4AP-HCl

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Cancer-treatment-induced biologicial and epigenetic signs of accelerated aging in cancer survivors: A systematic review

Alix Fastré, Charlotte Beaudart, Médéa Locquet
Public Health Aging Research & Epidemiology (PHARE) Group, Clinical Pharmacology Research Unit (URPC), Department of Biomedical Science, University of Namur (UNamur)
Email of presenting author: medea.locquet@unamur.be

With growing populations of cancer survivors, late effects of cancer treatments became a major public health burden. Emerging evidence suggests that cancer treatments may induce biological alterations consistent with an accelerated aging hypothesis; however, fragmented.
This systematic review (SR) aimed to synthesize biological biomarkers of treatment-induced accelerated aging in cancer survivors (CS) vs. cancer-free individuals.
The SR was conducted according to PRISMA guidelines. Databases (Scopus, PubMed) were searched (September 2025) to identify observational studies assessing biological or epigenetic aging biomarkers in cancer survivors exposed to cancer treatments. Eligible studies should also include a cancer-free comparison group. Aging biomarkers comprised inflammatory markers, immune cell phenotypes, telomeres, mitochondrial or DNA damage, and epigenetic clocks. Study selection, data extraction, and quality assessment were performed by 2 reviewers. When appropriate, pooled effect estimates were computed, and sensitivity analyses were conducted.
Of the 11,006 screened references, 22 studies were included. The most frequently reported biomarkers were inflammatory markers, immune cell phenotyping, circulating microRNAs, and epigenetic DNA methylation clocks. The references included were mainly cross-sectional or retrospective cohort studies, with sample sizes ranging from 38 to 2,000 CS. Most cohorts included childhood CS (n = 9) and breast CS (n = 8), with sex-specific or mixed populations, depending on cancer type. In pooled analyses, (hs)CRP was significantly higher in CS (k = 7; n = 15,544 individuals; standardized mean difference (SMD) = 1.06, 95% confidence interval (CI): 0.23-1.88; p = 0.012; I^2 = 97.7%), and epigenetic age acceleration was also higher (k = 3 cohorts; 7 effect sizes; n = 2,607 individuals; SMD = 0.31, 95% CI: 0.15-0.48; I^2 = 84.2%) vs. cancer-free controls. Heterogeneity between studies was high. Consistent patterns were observed in subgroup (chemotherapy vs. chemoradiotherapy; childhood vs. adult) and leave-one-out analyses, confirming the robustness of significant pooled effects.
This SR identified biological and epigenetic signs consistent with accelerated aging in CS from clinical studies. Major gaps include limited prospective data, heterogeneous methodologies, and underrepresentation of non-chemotherapy treatments. Standardized biomarkers are needed to support precision oncology, optimize treatment, prevent aging morbidities, and allow healthy aging in CS.

AI-guided competitive docking for virtual screening and compound efficacy prediction

Manon Mirgaux[1], Valeria Barcelli[2], Adeline C.Y. Chua[3], Pablo Bifani[2,3*], René Wintjens[1*]*

Abstract:

Machine learning has profoundly transformed the prediction of protein structures and interactions. In structure-based drug discovery, virtual docking has long been the standard approach, but a breakthrough emerged with the advent of co-folding generative models, giving rise to powerful tools such as RoseTTAFold All-Atom and AlphaFold3 (AF3). These methods can model protein–ligand interactions across a wide and largely unrestricted diversity of ligand types.

A key limitation, however, is that machine-learning-based docking methods generally generate an interaction pose for any ligand, independent of whether it truly binds or is inactive. While many models offer scoring functions to rank predicted complexes, reliably estimating binding affinities remains challenging. This raises two fundamental questions: (i) how can true binding events be differentiated from false positives? and (ii) how can predicted poses be ranked in a manner that accurately reflects their expected binding strengths? Addressing these questions constitutes the central motivation of this work.

In this work, we demonstrate that denoising diffusion–based co-folding approaches—such as AlphaFold3 and Boltz-1/2—achieve not only high accuracy in predicting protein–ligand interactions but also enable discrimination between active and inactive compounds. We propose a simple and efficient strategy, termed pairwise competitive docking, which ranks candidate molecules by directly comparing their relative binding at a protein's target site. When applied to 17 benchmark protein systems, this approach produced rankings consistent with experimental observations.

Furthermore, we demonstrate that pairwise competitive docking can accelerate the identification of promising hits from large chemical libraries and facilitate the de novo design of inhibitors with improved predicted potency. Overall, these results illustrate how modern machine-learning models can render structure-based drug discovery faster, more robust, and more cost-effective than approaches relying solely on experimental workflows.

Targeting ferroptosis resistance to sensitise cancer cells to radiotherapy/protontherapy

OPELE-NAVENGE Keïla1, SOUNNI Nor Eddine2, HEUSKIN Anne-Catherine1

[1]Namur Research Institute for Life Sciences (NARILIS), Laboratoire d'Analyse par Réaction Nucléaire (LARN), University of Namur (UNamur), Belgium

[2] Cancer Metabolism and Tumor Microenvironment Group, GIGA Cancer, Liège University, Belgium.

keila.opele@unamur.be

1. Context:

During radiotherapy or proton therapy, ionizing radiation induces direct DNA damage and indirect cellular damage through generation of reactive oxygen species (ROS). In the presence of ferrous ions (Fe^{2+}), ROS levels increase via Fenton reactions, promoting extensive lipid peroxidation and the accumulation of "lipid-ROS." When these lipid peroxides accumulate beyond the cell detoxification capacity, membrane integrity is lost, triggering ferroptosis, an iron-dependent cell death pathway. However, innate or acquired radioresistance still limits treatment efficacy and contributes to relapse. Therefore, a deeper understanding of the molecular mechanisms underlying radiotherapy resistance is essential to develop effective combination strategies to eradicate solid tumors.

2. Methods:

Four NSCLC cell lines (A549, H460, H1299, H195) were exposed to increasing X-ray doses or treated with ferroptosis inducers/inhibitors. First, we assessed the cell lines sensitivity to X-ray irradiation by clonogenic assays with or without an iron chelator. Then, expression levels of key ferroptosis markers involved in lipid biogenesis or in the antioxidant pathway of lipid-ROS were evaluated following irradiation or treatment with ferroptosis inducer or inhibitor. We also studied the enzymatic activity of TrxR, known to collaborate with GPX4 to detoxify lipid-ROS. Finally, we observed lipid peroxidation under the microscope following 0 Gy, 2 Gy or treatment with ferroptosis inducers.

3. Results:

Each cell line showed distinct sensitivity to X-ray exposure with A549 being the most resistant. These differences may relate to p53 status and/or differential expression of ferroptosis-related genes. Proteomic analyses also revealed potential biomarkers of resistance, which we will further investigate as possible therapeutic targets to enhance ferroptosis sensitivity. We will additionally sensitise ferroptosis-resistant cells by targeting proteins identified in the proteomic analysis, and we will test these strategies in combination with gold nanoparticles (GNPs), which are known to disrupt redox homeostasis.

Iron Based Photosensitizers Anchored on Metal Oxide Thin Films for a Greener Future

Lakshmi Narayan SATHEESH BABU
Ludovic TROIAN-GAUTIER
UCLouvain-IMCN-MOST
lakshmi.satheesh@uclouvain.be

Meeting global energy demands through sustainable energy production remains a critical challenge, as fossil fuel-based energy sources are unsustainable. Solar energy harvesting presents a promising solution to address both current and future energy needs. Our work focuses on solar energy conversion using Dye Sensitized Photoelectrochemical Cells (DSPECs), an advanced photoelectrochemical system designed to transform solar energy into chemical energy, primarily through water splitting to generate valuable products such as solar fuels [1]. Most of the DSPECs today still rely on noble metal complexes such as Ru (II) photosensitizers. In this work, we are focusing on the development of iron-based photosensitizer [2] as a sustainable alternative to the Ru(II) champion photosensitizers [3]. These newly formed Fe (III) photosensitizers [2, 4] were functionalized with anchoring groups that included phosphonic acid, silane, carboxylic acid (benzoic acid and isophthalic acid).
These photosensitizers were anchored on selected metal oxides, such as TiO_2, SnO_2, nanoITO and NiO. The resulting photoelectrodes were analyzed using various spectroscopic techniques, including UV-Vis absorption spectroscopy, steady-state and time-resolved luminescence, Spectro electrochemistry, ultrafast transient absorption spectroscopy and photocurrent measurements. These analyses provide crucial insights into the photophysical and electrochemical properties of these individual photoelectrodes, representing the first step in the development of novel DSPEC systems for sustainable energy applications. Our work represents a significant step toward paving the way for environmentally friendly solar energy conversion technologies. By advancing the understanding of Fe (III) photosensitizers and their interaction with semiconductor materials, we contribute to the broader goal of developing efficient, low-cost and sustainable DSPEC systems for solar fuel applications.

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Synthesis of new beta-lactams analogues designed for the detection of antimicrobial bacterial resistance by electrochemistry

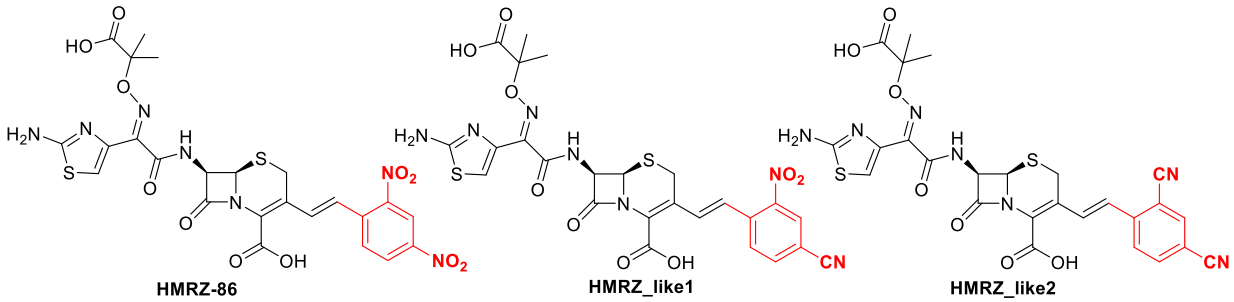
Jozie Tientcheu[a,b], Arnaud Beaufays[a,b], Mallory Draye[b], Pascal Mertens[b], Stéphane P. Vincent[a]

[a]Laboratoire de Chimie Bio-Organique (CBO),
University of Namur, Rue de Bruxelles 61, 5000 Namur, Belgium
[b]Coris BioConcept,
Rue Guillaume Fouquet 11, 5032 Gembloux, Belgium
jozie.tientcheu@unamur.be

The main class of antibiotics used to fight bacterial infectious diseases are β-lactams [1,2]. Unfortunately, bacterial resistance to drugs is rapidly acquired and disseminated which poses a significant threat to public health [3]. This underlines the fact that it is crucial to detect very early and accurately the antimicrobial resistance mechanism before administration of treatment to the patient [4].

The third-generation cephalosporin analogue HMRZ-86 is a substrate for some β-lactamases, and its hydrolysis product can be detected by electrochemical methods. Therefore, this molecule appears to be a good candidate for a use in an electrochemical test intended to detect β-lactamase activity. However, HMRZ-86 presents poor stability over time. The goal of the study was to modify the 2,4-dinitrostyryl moiety from this molecule and to evaluate the impact of these changes on the stability response of the new molecules.

For the synthesis of these various analogues, a common intermediate was used. The key synthetic step was a Wittig reaction.



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Synthesis of carbon-based bifunctional Lewis/Brønsted acid catalysts for 5-HMF production from cellobiose

Alessia Tonelli[a)], Richa Tomer[a)], Anthony Morena[b)], Luca Fusaro[b)], Carmela Alprile[b)], Sophie Hermans[a)]

a) MOST, Institute of Condensed Matter and Nanosciences, UCLouvain

b) NISM, Chemistry Department, UNamur

alessia.tonelli@uclouvain .be

Lignocellulosic biomass represents a valuable renewable feedstock for the synthesis of numerous green chemicals. Among the possible products that can be obtained from its degradation, 5-hydroxymethylfurfural (5-HMF) is a high added-value platform molecule that can be recovered from its cellulosic component via a three-step reaction promoted by both Brønsted and Lewis acid sites (Figure 1) [1]. In this study, we present a straightforward approach to synthesize efficient bifunctional catalysts by grafting benzyl sulfonic moieties (Brønsted sites) onto a carbon support (SX+ from NORIT, fraction < 50µm) functionalized with aluminosilicate patches (Lewis sites) grown from the precursor di-sec-butoxyaluminoxytriethoxysilane [2]. The resulting bifunctional catalysts (Figure 2) were extensively characterized and their catalytic performance investigated for the upgrading of cellobiose to 5-HMF. Bifunctional catalyst I4@BATEOS/SO_3H, with an average pore size of 45.8 Å and a total acidity of 1.25 mmol g^{-1}, was found to be the best performing material, yielding 37% of 5-HMF out of a 96% conversion of the initial cellobiose feed when tested over 23 h at 423 K in a designed solvent mixture. No significant side products were observed after 23 h, confirming the high selectivity of the catalyst.

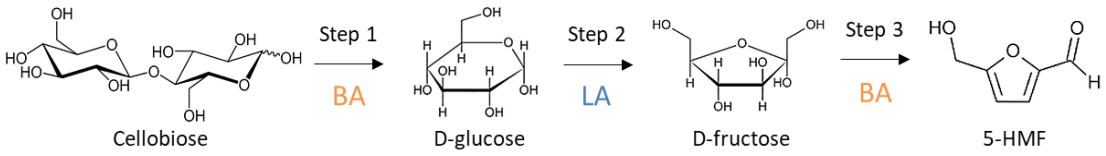

Figure.1 Synthesis of 5-hydroxymethylfurfural from cellobiose.

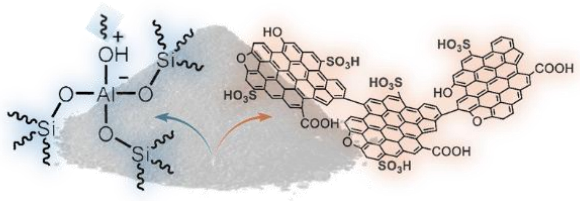

Figure.2 Structure of the bifunctional carbon-based catalysts.

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Molecular dynamics simulations of the first stage of the cathode manufacturing process

Marie Rose YOUBI KEMMOGNE, Arpit MISHRA, Giuliana MATERZANINI, Gian-Marco RIGNANESE
UCLouvain – IMCN – MODL
rose.youbi@uclouvain.be

Rechargeable Li-ion batteries (LIBs) have been widely used in various applications since their introduction by Sony in 1991. Known for their superior energy density, minimal memory effect, and long lifespan, LIBs are essential not only for portable electronics (e.g., mobile phones, medical devices, laptops) but also for providing green energy and meeting the growing demand for electricity. As a result, developing strategies that incorporate new materials and optimize the manufacturing process is crucial to reducing battery costs while maintaining performance and durability. In this context, computational simulation tools can be very useful, potentially reducing time, labor, and material costs [1]. Recently, a coarse-grained molecular dynamics (CGMD) approach was used to simulate Nickel-Manganese-Cobalt-based (NMC) cathodes (in particular, NMC111) [2]. In this poster, I will present our recent work simulating the first stage of the NMC811 cathode manufacturing process, namely, the preparation of the slurry, using this CGMD approach [2]. Due to the multicomponent and multi-scale nature of the slurry, the slurry components are treated in a rather crude way, with the active material treated as a collection of spherical particles with a specific density and size distribution. The carbon additive, binder, and solvent are combined into a "carbon-binder domain" (CBD), which is represented as a collection of identical effective spheres with the same density. We perform equilibrium CGMD simulations in the NPT ensemble to obtain the equilibrium density of this coarse-grained system. For this, we use a combination of force field (FF) parametrized on NMC111 experimental data [2]. With the same FF, we calculate the viscosity, a key rheological property of the slurry [3], using non-equilibrium MD simulations (NEMD) under shear at selected shear rates. The results for density and viscosity will be used to obtain a refined parametrization of the FF, based on in-house experimental data for NMC811. This will be achieved using both standard and machine-learning-based optimization techniques.

Keywords: Battery, manufacturing process, electrodes, slurry, coarse-grained molecular dynamics, machine-learning.

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