UMR 7140 Day 2025

Chimie de la Matière Complexe

Chemistry of Complex Matter

Date: 6th May 2025, from 9:00 onwards

Location: *Présidence de l'université de Strasbourg*

Alain Beretz Amphitheater New Patio

Access location

https://www.google.com/maps/place//data=!4m2!3m1!1s0x4796c8fe08475a2d:0xfb218506b2d98637?sa=X&ved=1t:8290&ictx=111

9:00 – 9:10	Opening Remarks and Introduction - UMR Day 2025	
9:10 – 9:25	**Julie Obeid** Systems Chemistry Laboratory *'Understanding the Splitting Mechanism of Coacervates Under an Electric Field'*	Session 1: Svetlana Samokhvalova
9:25 – 9:40	**Almaz Gilmullin** Chemoinformatics Laboratory *'Leveraging Generalized Condensed Graphs for Strategic Clustering of Retrosynthetic Pathways'*	
9:40 – 10:00	**Alexandre Locher** Laboratory of Mass Spectrometry of Interactions and Systems *'Structural analysis of antimicrobial peptides by chemical cross-linking coupled to mass spectrometry in liposomal environment'*	
10:00 – 10:10	**Jorge Hilari** French Chemical Society	
10:10 – 10:40	Coffee Break	
10:40 – 11:00	**Matt Ball** Chemoinformatics Laboratory *'Reaction Condition Prediction in CASP: A Critical Perspective on Data and Methodology'*	Session 2: Raaif Siddeeque
11:00 – 11:15	**Ashini Shah** Laboratory of Bioelectrochemistry and Spectroscopy *'Detection of Microplastics in Human Tissue Using FTIR Microspectroscopy*	
11:15 – 11:30	**Mark Ely Namoro** Molecular Modelling and Simulation Laboratory *'Study of the dynamics and proflavine host-guest binding of a bis-acridinium tweezer system'*	

11:30 – 11:50	**Raaif Siddeeque** Laboratory of Bioelectrochemistry and Spectroscopy *'Proton uptake in cytochrome bd-I from E.coli: electrocatalytic and spectroscopic investigations'*	
11:50 – 14:00	Lunch Break	
14:00 – 14:20	**Aykhan Israfilli** Chemoinformatics Laboratory *'Meta-Benchmarking study of Docking Protocols'*	Session 3: Pham David Jérôme
14:20 – 14:40	**Lola Alez-Martin** Laboratory of Mass Spectrometry of Interactions and Systems *'Advanced characterization of monoclonal antibodies charge variants using capillary electrophoresis and tandem mass spectrometry'*	
14:40 – 15:00	**Eliott Jung** Molecular Modelling and Simulation Laboratory *'Synthesis of bioinspired complex polycyclic motifs supported by DFT mechanistic studies'*	
15:00 – 15:45	Coffee Break	
15:45 – 16:05	**Malak Jaber** Systems Chemistry Laboratory *'Controlling the Self-assembly and Crystallization in Stimuli-Responsive Coacervate Microcompartments'*	Session 4: Almaz Gilmullin
16:05 – 16:25	**Jules Wolff** Molecular Modelling and Simulation Laboratory *'Cations Effect on Pt Electrodes in Alkaline HER Conditions Studied by Molecular Dynamics at Constant Potentials'*	
16:25 – 16:40	**Pauline André** Laboratory of Synthesis and Functions of Molecular Architectures *'Covalent-organic frameworks synthesized in deep eutectic solvents'*	
16:40 – 16:50	Conclusion of the UMR 2025 day	

Understanding the Splitting Mechanism of Coacervates Under an Electric Field

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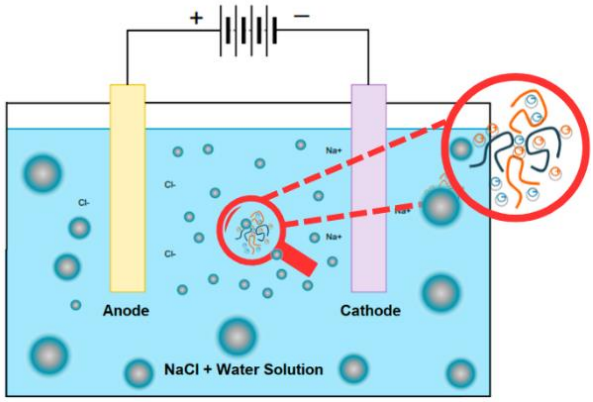
Keywords: Coacervates, splitting, electric field, coacervate emulsions…

Complex coacervates are droplets spontaneously formed via liquid-liquid phase-separation when oppositely charged polyelectrolytes interact in water.[1] These droplets, rich in polymers yet immiscible with their surrounding aqueous environment, enable membranelles compartmentalization.[2] Their unique properties make them ideal for applications such as drug delivery and protocell models.[3] However, the applications of coacervate emulsions / droplets are limited by their fast coalescence, due to low surface tension.[4] Recently, we have discovered that coacervates can split in weak electric fields, leading to coacervate emulsions that are stable against coalescence. However, the mechanism of this splitting remains undetermined.

In this project, we systematically study different factors that influence the splitting: such as the ionic strength of the system, the chemical nature and molecular weight of the polyelectrolytes, and the strength of the electric field. By studying the effect of such parameters in the splitting, we can uncover new mechanistic information about this new behavior, as well as predicting and controlling it. This allows for novel approaches towards spatial control over coacervate materials. Moreover, understanding the mechanisms of coacervate splitting leads to better understanding of such complex systems.



Scheme 1: Splitting of the coacervates in the electric field between two electrodes.

Acknowledgements. *Thanks to the CSC Graduate School funded by the French National Research Agency (CSC-IGSANR-17-EURE-0016) for a Master fellowship.*

(1) Yewdall, N. A.; André, A. A. M.; Lu, T.; Spruijt, E. *Current Opinion in Colloid & Interface Science* **2021**, *52*, 101416.
(2) Deng, N.-N. *Biomicrofluidics* **2020**, *14* (5), 051301.
(3) Ivanov, T.; Doan-Nguyen, Thao. P.; Belahouane, M. A.; Dai, Z.; Cao, S.; Landfester, K.; Caire da Silva, L. *Macromol Rapid Commun* **2024**, *45* (24), 2400626.
(4) Lin, Z.; Beneyton, T.; Baret, J.-C.; Martin, N. *Small Methods* **2023**, *7* (12), 2300496.

Leveraging Generalized Condensed Graphs for Strategic Clustering of Retrosynthetic Pathways

Almaz Gilmullin[a], Tagir Akhmetshin[a], Timur Madzhidov[b], Alexandre Varnek[a]

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Keywords: CASP, retrosynthesis, synthetic routes clustering, strategic bonds

Modern computer-aided synthesis planning (CASP) platforms now routinely generate multiple plausible routes to a target molecule using advanced AI-driven retrosynthetic algorithms [1]. However, evaluating and comparing these predicted routes remains challenging, as conventional metrics (e.g., step count, yield, or accuracy against known routes) cannot capture partial similarities or strategic differences among distinct routes [2, 3]. To address this gap, we developed a graph-based approach for route comparison based on Condensed Graph of Reaction (CGR) representations. A CGR merges all reactants and products of a chemical transformation into a single graph (a “pseudo-molecule”) that encodes bond-breaking and bond-forming reactions [3]. We extend this concept to multi-step syntheses with two complementary route descriptors: a Generalized CGR (G-CGR) that captures all changes (including leaving groups and reagents) across the entire pathway, and a Reduced Generalized CGR (RG-CGR) that considers only “strategic bonds” - bonds formed between atoms that are present in the final target molecule. Morgan circular fingerprints are then generated from these graph representations to provide numerical descriptors for each route, and hierarchical clustering of these fingerprints groups chemically similar routes together. This graph-based methodology enables a more nuanced and intuitive comparison of CASP-generated pathways, effectively clustering redundant solutions and highlighting distinct strategic alternatives beyond the reach of existing techniques. Both G-CGR and RG-CGR are implemented and available in the previously developed by our group SynPlanner retrosynthesis tool [5].

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Structural analysis of antimicrobial peptides by chemical cross-linking coupled to mass spectrometry in liposomal environment

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[2] Laboratoire de Biophysique des Membranes et RMN, UMR 7177

Antimicrobial peptides (AMPs) are short, membrane-active peptides, naturally present in most organisms playing a crucial role in the defense of the host against bacterial pathogens, and they reduce the risk of resistance development. A lot of studies have shown that they are able to kill bacterial pathogens by permeabilising their membrane, making them an attractive alternative to treat multiresistant bacteria [1,2].

PGLa and Mag2 are cationic amphipathic antimicrobial peptides belonging to the magainin family. Both are found in the skin of the African frog *Xenopus laevis* and adopt an α-helix structure when in contact with a phospholipid bilayer. It has been shown that they selectively affect bacterial membranes by acting parallel to the bilayer surface, and that mixtures of PGLa/Mag2 exhibit synergistic improvement in antimicrobial activity [3,4]. To gain better understanding of the interaction mechanism of these two peptides in relation with synergism, we are developing a chemical cross-linking coupled to mass spectrometry approach in a membrane-mimicking environment (DDM detergent and phospholipid liposomes). Cross-linking agents such as DSS or DSG are used to covalently link the peptides through their lysine residues (K) if those are sufficiently close in space. During my mastership, we monitored the formation of a covalently cross-linked PGLa/Mag2 heterodimer after incorporating the peptides into liposomes composed of POPE:POPG and DMPE:DMPG. The cross-linking efficiency as well as the peptide stoichiometry were monitored and optimized by MALDI-MS.

Once the optimal conditions for obtaining a PGLa/Mag2 heterodimer have been determined, these cross-linked peptides are analyzed by nanoLC-MS/MS to obtain detailed structural information, particularly regarding their spatial proximity.

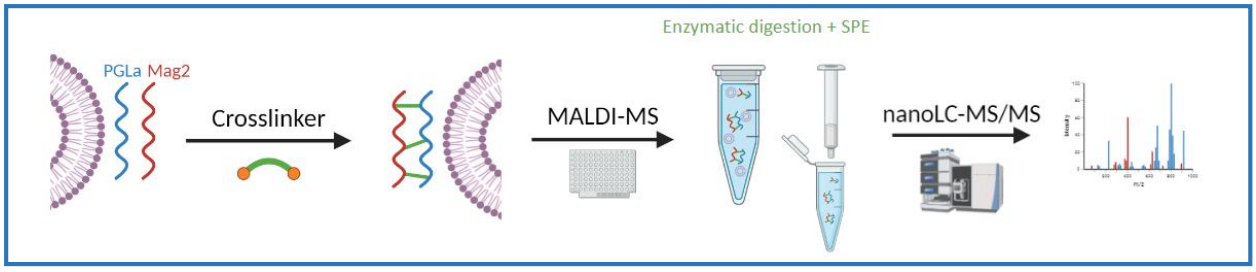

Figure 1: Workflow of the chemical cross-linking reaction with PGLa and Mag2 coupled to mass spectrometry, created in Biorender.com

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(2) Finger, S. Interaction of Cyclic Antimicrobial Hexapeptides with Model Lipid Membranes, Universitäts- und Landesbibliothek Sachsen-Anhalt, 2021, p 1 Online-Ressource (239 Seiten). https://doi.org/10.25673/39656.
(3) Harmouche, N.; Bechinger, B. Lipid-Mediated Interactions between the Antimicrobial Peptides Magainin 2 and PGLa in Bilayers. *Biophysical Journal* **2018**, *115* (6), 1033–1044. https://doi.org/10.1016/j.bpj.2018.08.009.
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Reaction Condition Prediction in CASP: A Critical Perspective on Data and Methodology

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Keywords: Cheminformatics, Computer-Aided Synthesis Planning

The selection of optimal reaction conditions is a critical challenge in synthetic chemistry, influencing the efficiency, sustainability, and scalability of chemical processes. While machine learning (ML) has emerged as a promising tool for predicting reaction conditions in computer-aided synthesis planning (CASP), existing approaches face many significant challenges, including data quality, sparsity and method evaluation. Recent studies have suggested that these models may fail to surpass literature-derived popularity baselines, calling into question the practical value of these models. In this work, we analyse the unique challenge of condition modelling compared to the modelling of other reaction properties, emphasising the importance of data quality, representation and appropriate method evaluation. We provide a critical review of state-of-the-art ML techniques, identifying innovations which have addressed the key challenges facing researchers when modelling conditions. To illustrate how relevant reaction representations can improve existing models, we perform a case study of heteroaromatic Suzuki-Miyaura reactions, derived from US patent data (USPTO). Using Condensed Graph of Reaction-based inputs, we demonstrate how this alternative representation can enhance the predictive power of a model beyond popularity baselines. We conclude by proposing actionable future directions, including data-centric approaches beyond simple curation, to support more robust and generalisable condition prediction models.

Detection of Microplastics in Human Heart Tissue Using FTIR Microspectroscopy

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Keywords: microplastics, heart tissue, microIR, chemical imaging

Microplastics have been identified as one of the most serious threats to the environment due to their prevalence across all ecosystems, including the human body. Since the discovery of microplastics in human placenta (Ragusa et al., 2021), research around microplastic detection in human tissues has expanded significantly. Microplastics have been identified in at least 15 different human samples, including heart tissue, lung tissue, feces, and blood. Several cell line studies suggest that microplastics are associated with a host of adverse effects, including the exacerbation of inflammatory processes (Kutralam-Muniasamy et al., 2023). Given the rising concerns about microplastic toxicity, we aim to identify microplastics in human heart tissue and determine whether their presence correlates with inflammation levels. We investigate cross-sections of the internal thoracic artery from 8 different patients with varying degrees of inflammation. FTIR microspectroscopy allows us to identify microplastics spectrally (rather than by eye, as in previous studies) and visualize their spatial distribution across the tissues. We begin by investigating the baseline composition of artery tissues so anomalies such as microplastics can be accurately identified throughout the project.

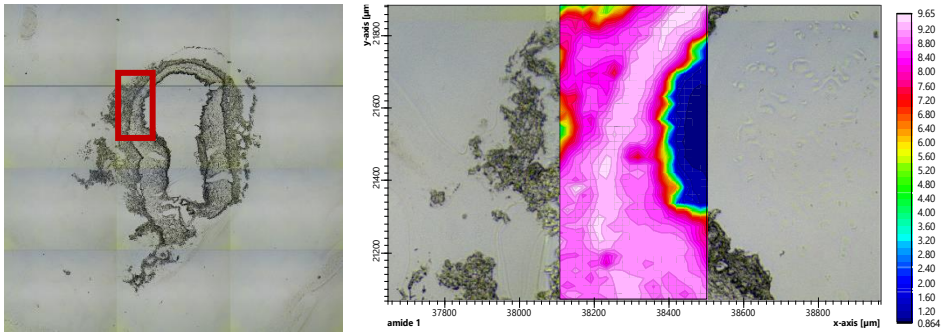

Figure 1. a) cross section of artery, with area of chemical mapping indicated. b) microIR chemical image of artery section, indicating changes in the Amide 1 integration.

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Study of the dynamics and proflavine host-guest binding of a bis-acridinium tweezer system

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Keywords: bis-acridinium tweezer, proflavine, host-guest chemistry, molecular dynamics

The selective extraction of polycyclic aromatic hydrocarbons is a challenge due to their similar physicochemical properties with their hydrogenated counterparts. Molecular encapsulation is a promising strategy to overcome this difficulty[1]. Work done by the LSAMM (Strasbourg) has demonstrated a selective response of a bis-acridinium tweezer to proflavine-like molecules. The proposed mechanism involves the hydroxylation of the tweezer upon the formation of a proflavine inclusion complex, followed by a second hydroxylation also presumed to be proflavine-assisted. The resulting bis-hydroxylated tweezer undergoes a spontaneous conformational change, ending in a single conformer seen through NMR experiments.

Following the experimental work, the conformational dynamics and host-guest interactions of a bis-acridinium system were investigated through molecular dynamics simulations. The tweezer was found to form a long-lasting exclusion complex with proflavine, supporting the proposed mechanism for the first hydroxylation event. The singly-hydroxylated tweezer was found to form exclusion complexes with proflavine with lifetimes depending on the presence or not of water in the system. The three key conformations of the bis-hydroxylated tweezer (named **u,s,w**) were investigated. Ramachandran plots and population analyses confirmed that the proposed conformations occupy most of the population during the simulation timescale. The conformer **w** seen in NMR experiments was revealed to have the lowest free energy via free energy and DFT calculations. Analysis of the potential energies showed that **w** was stabilized more by solute-solvent interactions compared to **u** and **s** due to the larger cavity size seen in **w.**

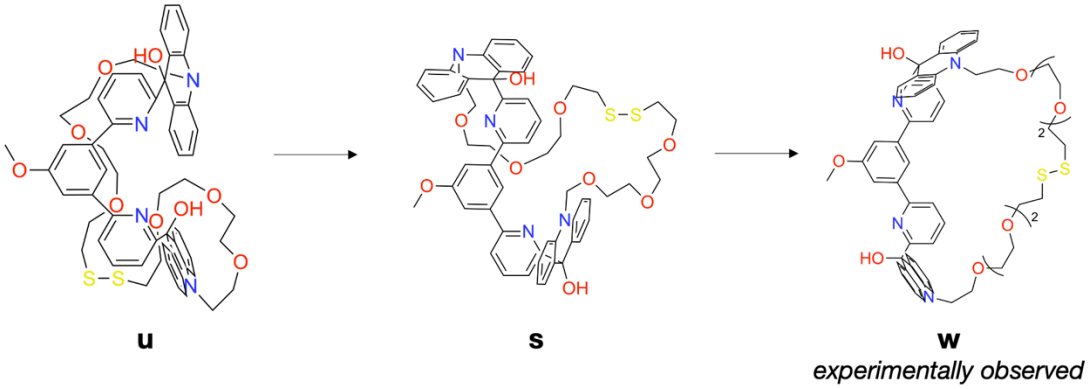

Figure 1. The conformational change of the bis-hydroxylated tweezer observed in molecular dynamics simulations.

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Proton uptake in cytochrome *bd* -I from *E. coli*: electrocatalytic and spectroscopic investigations

Raaif Siddeeque[1], Lucia Heger[2], Jan Kaegi[2], Daniel Wohlwend[2], Thorsten Friedrich[2], Frédéric Melin[1], and Petra Hellwig[1]

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Keywords: Bioelectrochemistry, Cytochrome *bd*-I, FTIR-spectroscopy.

The selective reduction of oxygen to water is crucial to life and a central process in aerobic organisms. It is catalysed by several different enzymes, including cytochrome *c* oxidases, found for example in mammals, and cytochrome *bd* oxidases that are solely present in prokaryotes. These essential enzymes also play a crucial role in protection against oxidative stress, in virulence, adaptability and antibiotic resistance. Electrochemical and spectroscopic studies allow obtaining information on the oxygen reduction, coupled protonation processes, and the interaction with small molecules that rule the signaling processes in the biological cell, including NO.[1-2]
Here we present the electrocatalytic study of these membrane proteins immobilized on nanostructured surfaces. Different modes of immobilization have been probed by infrared spectroscopy and the effect of the presence of lipids on the electrochemical reactivity of the membrane proteins has been analysed. Site-directed mutants at position D58 and nearby residues reveal that this residue is a crucial part of the proton path to the active site. It can be shown that the NO release kinetics is associated with proton uptake and thus with the oxygen reaction. First paragraph.

[1] Nikolaev, A.; Safarian, S.; Thesseling, A.; Wohlwend, D.; Friedrich, T.; Michel, H.; Kusumoto, T.; Sakamoto, J.; Melin, F.; Hellwig P. 'Electrocatalytic evidence of the diversity of the oxygen reaction in the bacterial bd oxidase from different organisms' Biochim. Biophys. Acta (2021) 1862, 148436.

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Meta-Benchmarking study of Docking Protocols

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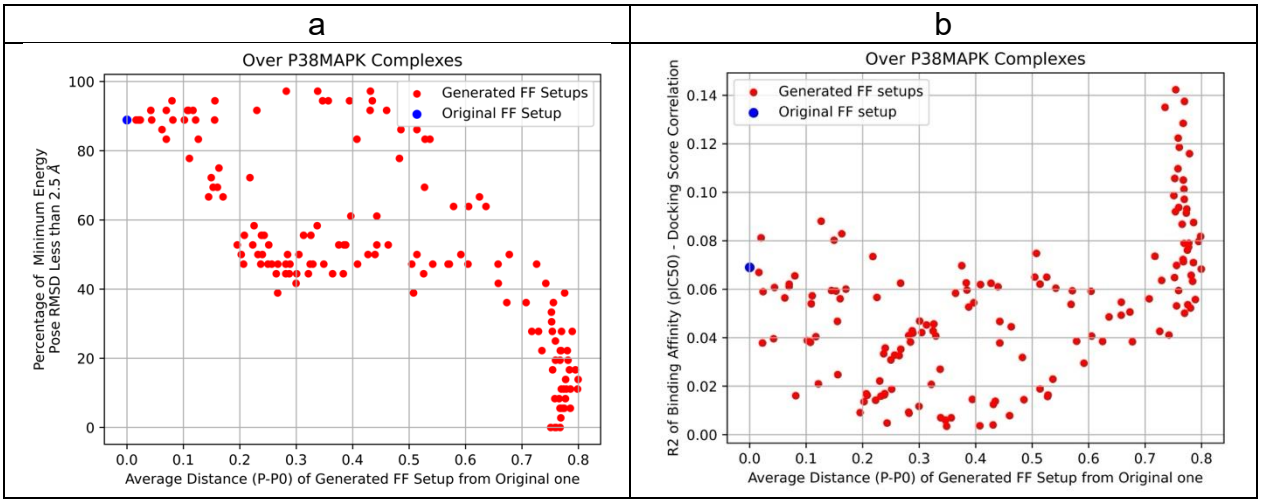
Keywords: Docking, Benchmarking, Calibration

Despite the wide-spread use of docking as a virtual screening tool, its performance is often disappointing. Since it is a well-known truth acknowledged by all practitioners of docking, and yet not visible from literature, it is reasonable to assert that there is a significant bias toward selectively publishing only success stories. Here, we wish to provide the auditory with detailed and pedagogical insight of the problems affecting the calibration and benchmarking procedures of docking algorithms. In addition to a thorough critical evaluation of the docking benchmark publications, we use our in-house tool S4MPLE for in depth exploration of its behaviour and performances with respect to the tunable energy function parameters. Our findings - likely applicable to any docking protocol suggest that it is relatively easy to calibrate the docking score to obtain native pose prediction results in redocking. While many different setups achieve the near-optimal results in this respect, those different setups show radically different ranking of the poses and ligands in terms of energy/affinity/score. Therefore, we suggest that an ideal docking calibration and benchmarking should always include a multi-objective optimization approach which includes both pose prediction and active compound retrieval criteria while adopting the as far as possible best-practices in it.



Performances of generated FF setups on pose ranking (a) and virtual screening (b) over P38MAPK complexes as an example

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Advanced characterization of monoclonal antibodies charge variants using capillary electrophoresis and tandem mass spectrometry

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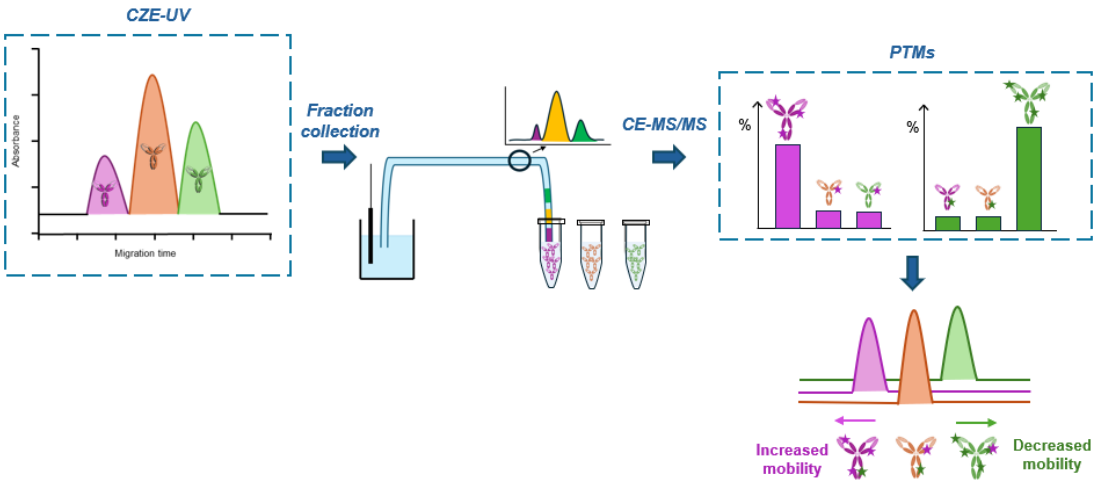
[1] Laboratoire de Spectrométrie de Masse des Interactions et des Systèmes (LSMIS) UMR 7140 (Unistra-CNRS), Université de Strasbourg, France.
[2] Université Paris Cité, Unité de Technologies Chimiques et Biologiques pour la Santé (UTCBS), CNRS UMR8258, Inserm U1022, Faculté des sciences pharmaceutiques et biologiques, Paris, France.

Monoclonal antibodies (mAbs) are therapeutic biomolecules that have known a huge success in the pharmaceutical industry the last 20 years. For instance, 21 therapeutic mAbs received their first approval in 2024[1]. However, these are structurally complex macromolecules and can undergo post-translational modifications (PTMs), potentially leading to the formation of charge variants.

Capillary Zone Electrophoresis (CZE) is particularly adapted for the separation of charge variants, however the selectivity provided by the method is not entirely understood. During this work, we first used CZE-UV to characterize infliximab charge variants of the innovator and biosimilar products. The CZE-UV analysis provided a specific electrophoretic separation of charge variants for each biosimilar. Enzymatic treatment of the antibodies allowed to attribute the charge variants to C-terminal lysine dissimilarities. The same strategy applied to pembrolizumab showed that none of the five charge variants separated were coming from N-glycans or C-terminal lysine residues.

Thus, an analytical strategy based on the fraction collection of the separated charge variants in CZE-UV for offline characterization in CE coupled to tandem mass spectrometry (MS/MS) was developed. CE-MS/MS allowed the identification of several PTMs such as pyroglutamate formation and deamidation from asparagine that could be correlated to a decreased mobility of the charge variants. For the first time, the formation of succinimide from aspartic acid could be successfully characterize using CE-MS/MS and was correlated to an increased mobility of the charge variants. CZE-UV separation resulted from the synergistic effect of several simultaneous PTMs affecting the apparent mobilities of the charge variants of pembrolizumab.



[1] Crescioli S, Kaplon H, Wang L, Visweswaraiah J, Kapoor V, Reichert JM. Antibodies to watch in 2025. mAbs. 2025 Dec 31;17(1):2443538. https://doi.org/10.1080/19420862.2024.2443538.

Synthesis of bioinspired complex polycyclic motifs supported by DFT mechanistic studies

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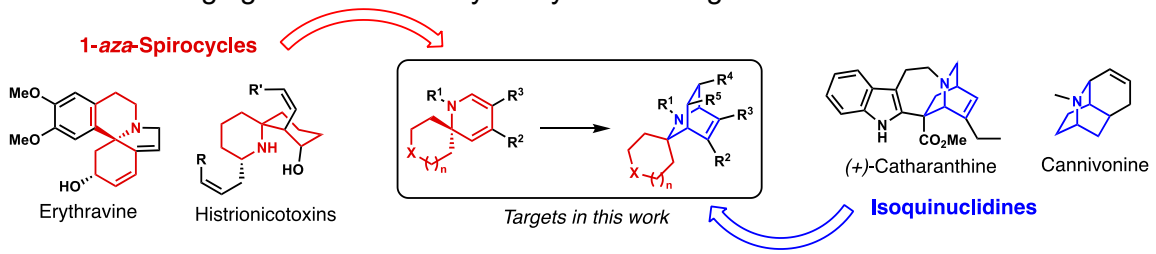
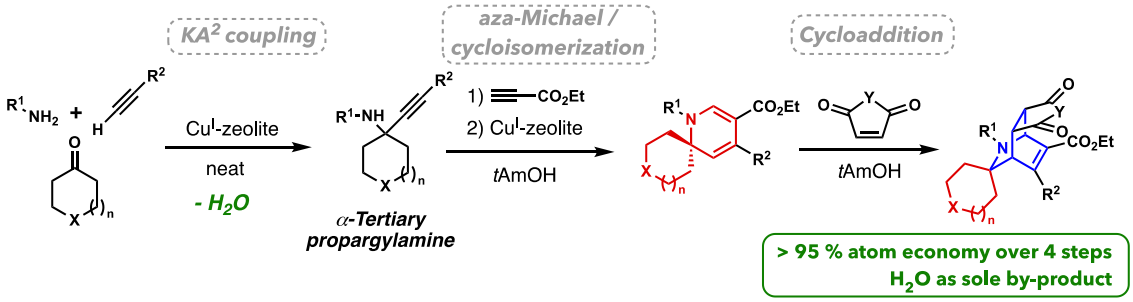
Keywords : Spirocyclic molecules ; Tridimentional complexity ; Green synthesis ; DFT calculations.

Constructing 3D *aza*-polycyclic architectures remains a big challenge in organic synthesis. In particular, much synthetic efforts have been devoted to **1-azaspirocyclic** and **isoquinuclidine** ring systems, due to their presence in many natural products of biological relevance (**Scheme 1**).[1,2] Our goal is to go further in 3D structural complexity by accessing to unprecedented architectures merging these two *aza*-cyclic systems of high relevance.



Scheme 1

Herein, we wish to report our synthetic approach towards this complex azaspiro/isoquinuclidine hybrid skeleton from simple starting materials (**Scheme 2**). Our approach starts with a 3-step sequence, including 2 steps under Cu^{I}-zeolite catalysis (*i.e.,* KA^2 coupling and enyne cycloisomerization reactions)[3], that first furnishes **1-azaspirocyclic** systems featuring a 1,2-dihydropyridine motif. The potential of the resulting 1,2-dihydropyridine motif as diene is finally exploited to construct the additional **isoquinuclidine** ring system *via* a formal cycloaddition process.[4] DFT calculations are conducted in parallel to rationalize the reaction mechanism and energetic pathway of the cycloaddition process. Noteworthy is that this methodology is highly atom and step economical, with water as sole by-product during the whole 4-step sequence.



Scheme 2

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Controlling the Self-assembly and Crystallization in Stimuli-Responsive Coacervate Microcompartments

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Keywords: Coacervates, self-assembly, crystallization, compartmentalization

Controlling supramolecular interactions is challenging, yet critical to many applications. Even for "simple" supramolecular architectures, self-assembly in non-optimal conditions can lead to multiple structures with different properties.[1] A similar case can be made for crystallization; for instance, forming protein crystals requires a non-trivial optimization of the conditions to obtain well-defined structures.[2,3] To facilitate these processes, we aim to develop new solvents where supramolecular interactions can be precisely tuned. Coacervates are liquid droplets that form spontaneously due to the interactions of a single polymer with itself or between two oppositely charged polyelectrolytes. They are aqueous, but they contain most of the polymer chains from the solution, which makes them relatively hydrophobic while containing a larger density of charges.[4] Due to this unusual combination of hydrophobicity and charges, coacervates solubilize most molecules. Both polar and apolar solutes are more soluble in the coacervate phase than in water, which leads to their spontaneous concentration and compartmentalization into coacervate droplets and their depletion from the rest of the solution.[5] In this study, we investigate how the unique environment within coacervates influences supramolecular self-assembly and crystallization, and study how the responsiveness of the coacervate phase translates to the compartmentalized structures. By tuning the ionic strength and polyelectrolyte composition, we explore how different properties of the coacervates affect crystalline nucleation and growth.

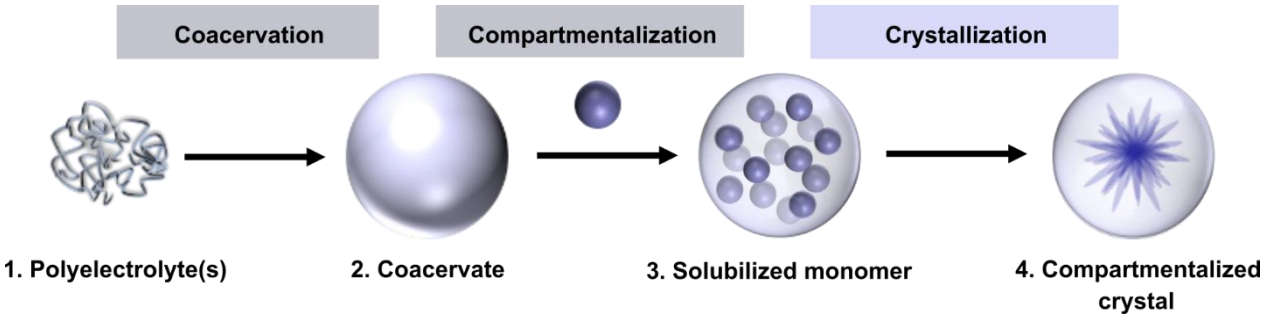

Figure 1. *Scheme illustrating the proposed strategy for achieving crystallization within coacervate compartments.*

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Cations Effect on Pt Electrodes in Alkaline HER Conditions Studied by Molecular Dynamics at Constant Potentials

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Rising interest for dihydrogen as an energy vector has been putting the hydrogen evolution reaction (HER) at the forefront of research. The HER has been highly studied and optimized at different scales: catalyst design, operating conditions (pH, temperature) and electrolyte. At the electrolyte level, the crucial role of the cations has been highlighted on Pt, hinting that their re-organization within the electrochemical double layer (EDL) may critically influence a given reaction kinetics [1]. A coherent mapping of the EDL structure can be obtained using “classical” molecular dynamics (MD) in order to rationalize this influence.

In 2020, the MetalWalls package [2] was developed in order to perform ‘all-atom constant potential MD’ and has been enabling a detailed mapping of the EDL. With the aim of unveiling the link between cations nature and the electrode/electrolyte properties, this study focuses on MD simulations at 0 and 1V on platinum monocrystalline facets. Different electrolytes (Aqueous solutions of 1M NaOH, KOH, CsOH) are investigated. Key properties such as the water distribution and its orientation as a function of the distance to the Pt surface as well as the cation concentration and their 1st shell solvation characteristics as a function of the distance to the Pt surface have been obtained, as illustrated in **Figure 1**, and the pivotal influence of the cation nature on these properties evidenced. The observed properties are then discussed in the light of experimental observations to correlate electrode/electrolyte interface properties and HER activity [3].

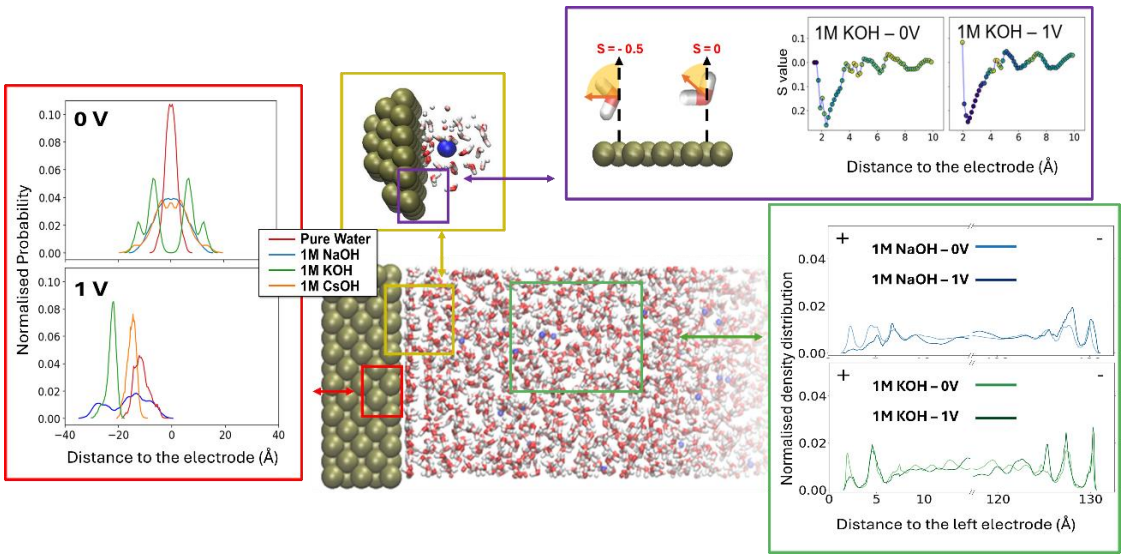

Figure 1 : Snapshot of the 1M NaOH system after 5 ns. Extracted data are presented as electrode charge for system with different cation types (red box), view of a solvated Na^+ near Pt(100) electrode (yellow box), orientation of water near the electrode measured through the orientation order parameters for K^+ systems (purple box), density profile of Na^+, and K^+ along the z axes of the box (green box). The simulation were performed at 0 and 1V during 10-20 ns in a box of 14nm long using the MetaWalls software.

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Covalent-organic frameworks synthesized in deep eutectic solvents

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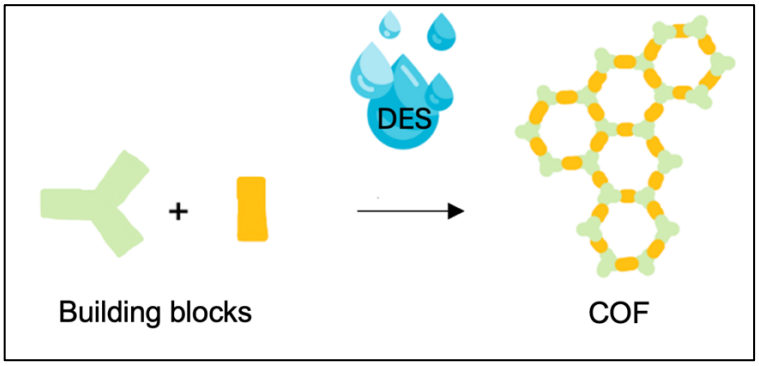
Keywords: Green Chemistry, porous materials, sustainable solvents

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

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



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