



Ráðstefna Efnís 2022

Efnafræði og umhverfið



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The Icelandic Chemical Society



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Efnafraeði og umhverfið

Ráðstefnudagskrá

	Fimmtudagur, 11. ágúst	Föstudagur, 12. ágúst
12:30-13:00	Skráning	
13:00-13:15	Setning	Fyrirlestrar
13:15-14:30	Fyrirlestrar	
14:30-14:45	Kaffi hlé	
14:45-16:00	Fyrirlestrar	
16:00-17:00	Veggspjaldakynningar	
19:00-22:00		Ráðstefnukvöldverður

Fimmtudagurinn 11. ágúst, 2022

- 12:30-13:05 **Skráning**
- 13:05-13:15 **Setning**
- 13:15-13:50 **Jón Ólafsson** – *The North Atlantic CO₂ sink*
- 13:50-14:10 **Ómar Freyr Sigurbjörnsson** – *E-fuels: past, present and future*
- 14:10-14:30 **Camila Pía Canales** – *The decade of hydrogen: where are we heading to?*
- 14:30-14:45 **Kaffi hlé**
- 14:45-15:20 **Steinar Birgisson** - *FeSi production in Iceland – Environmental impact and how to improve*
- 15:20-15:40 **Sara Jónsdóttir Glaser** – *Wheat bran-based biorefinery: Extracting bran components through fractionation based on steam explosion and hydrotropic extraction*
- 15:40-16:00 **Luis Antonio G. Arana Olivari** – *Brush polymers with cyclic and/or divalent side chains*
- 16:00-17:00 **Veggspjaldakynning 1**

Föstudagurinn 12. ágúst, 2022

- 13:00-13:35 **Fatemeh Hanifpour** – *Are transition metal nitrides suitable electrocatalysts towards the nitrogen reduction reaction?*
- 13:35-14:10 **Anna Bergljót Gunnarsdóttir** - *Screening of transition metal nitrides as electrocatalysts for nitrogen reduction using operando ammonia quantification*
- 14:10-14:30 **Yiming Yang Jónatansdóttir** – *Exploring the prevalence of weak allosteric effectors in non-allosteric metabolic enzymes*
- 14:30-14:45 **Kaffihlé**
- 14:45-15:20 **Már Másson** - *Synthesis of chitosan derivatives and structure-antimicrobial activity studies*
- 15:20-15:40 **Sreejith S. Jayabhavan** – *Crystal habit modification of metronidazole by supramolecular gels with complementary functionality*
- 15:40-16:00 **Younes Abghoui** – *Electrocatalysis for Green Production of Hydrogen*
- 16:00-17:00 **Veggspjaldakynning 2**
- 17:00-19:00 **Hlé**
- 19:00-22:00 **Ráðstefnukvöldverður**





FÍN

Félag íslenskra náttúrufræðinga

Fínasta stéttarfélagið

Chemistry and the Environment

Conference Program

	Thursday, August 11th	Friday, August 12th
12:30-13:00	Registration	
13:00-13:15	Welcome announcement	Oral presentations
13:15-14:30	Oral presentations	
14:30-14:45	Coffee break	
14:45-16:00	Oral presentations	
16:00-17:00	Poster session	
19:00-22:00		Conference dinner

Thursday, August 11th, 2022

- 12:30-13:05 **Registration**
- 13:05-13:15 **Welcome announcements**
- 13:15-13:50 **Jón Ólafsson** – *The North Atlantic CO₂ sink*
- 13:50-14:10 **Ómar Freyr Sigurbjörnsson** – *E-fuels: past, present and future*
- 14:10-14:30 **Camila Pía Canales** – *The decade of hydrogen: where are we heading to?*
- 14:30-14:45 **Coffee break**
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- 15:40-16:00 **Luis Antonio G. Arana Olivari** – *Brush polymers with cyclic and/or divalent side chains*
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- 15:40-16:00 **Younes Abghoui** – *Electrocatalysis for Green Production of Hydrogen*
- 16:00-17:00 **Poster session 2**
- 17:00-19:00 **Break**
- 19:00-22:00 **Conference dinner**





Er um við að leita að þér?

Elkem auglýsir eftir öflugum og hæfileikaríku fólki í tvær stöður innan fyrirtækisins

Leiðtogi Eldfast

Starfið felur í sér sérhæfingu á sviði eldfastra efna (refractory materials). Við leitum eftir einstaklingi sem hefur þekkingu á efnafræði og hefur góða greiningarhæfni. Starfið er stjórnunarstarf sem fellst í að leiða hóp í framleiðslu og viðhaldi á eldföstum búnaði fyrir verksmiðjuna.

Menntunar- og hæfniviðmið

- Háskólamenntun sem nýtist í starfi, t.d. efnafræði eða aðrar raungreinar.
- Reynsla af stjórnunarstörfum æskileg.
- Frumkvæði, stjórnendahæfileikar og sjálfstæð vinnubrögð.
- Vilji og geta til að vinna í krefjandi aðstæðum.
- Góð öryggisvitund og jákvætt viðhorf.
- Öguð og nákvæm vinnubrögð ásamt stundvísi.

Ferilseigandi Rannsóknar

Starfið felur í sér almennt gæðaeftirlit og umbætur á gæðasviði rannsóknarstofu við efnagreiningar á FeSi málmi og hráefnum tengdum framleiðslunni. Við leitum eftir einstaklingi sem hefur m.a. hæfni í skipulagningu og þróun ásamt viðhaldi og innleiðingu tækjabúnaðar.

Menntunar- og hæfniviðmið

- Háskólamenntun sem nýtist í starfi, t.d. raungreinar.
- Reynsla úr sambærilegum störfum t.d. rannsóknarstofum.
- Vilji og geta til að vinna í krefjandi aðstæðum.
- Góð öryggisvitund og jákvætt viðhorf.
- Frumkvæði og sjálfstæð vinnubrögð.
- Öguð og nákvæm vinnubrögð ásamt stundvísi.

Elkem á Íslandi er hluti af sterki alþjóðlegri heild, Elkem ASA, sem er einn af helstu framleiðendum heims á kísilafurðum. Áherslur fyrirtækisins er að hafa fjölbreytileikann að leiðarljósi og eru einkunnarorð okkar þátttaka, nákvæmni, virðing og stöðugar framfarir.

Elkem Ísland er traustur og eftirsóknarverður vinnustaður og hentar öllum, óháð kyni. Vakin er athygli á því að Elkem er vímuefnalaus vinnustaður.

Sótt er um rafrænt á ráðningarvef Elkem á www.elkem.is eða með því að skanna QR kóðann hér til hliðar.

Umsóknarfrestur er til og með 29. ágúst 2022



Skannaðu mig

Fyrirlestrar
Oral presentations

The North Atlantic CO₂ sink

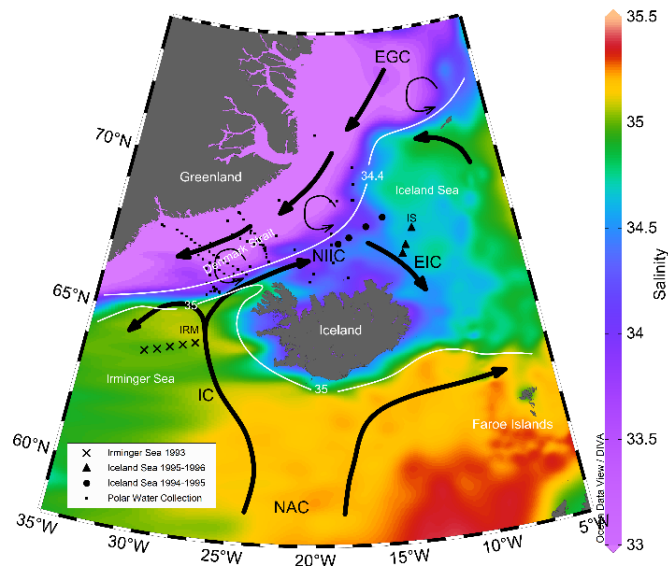
Jón Ólafsson¹ and Sólveig Rósa Ólafsdóttir²

¹Institute of Earth Sciences, Sturlugata 7 Askja, University of Iceland, 101 Reykjavik, Iceland

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ABSTRACT

The North Atlantic north of 50°N is one of the most intense ocean sink areas for atmospheric CO₂ considering the flux per unit area, 0.27 Pg-C yr⁻¹, equivalent to -2.5 mol C m⁻² yr⁻¹. This is on account of processes which sustain CO₂ air-sea fluxes. The region is in the northern limb of



the Global Thermohaline Circulation, a path for the long term deep sea sequestration of carbon dioxide. The surface water masses in the North Atlantic are of contrasting origins and character, on the one hand the northward flowing North Atlantic Drift, a Gulf Stream offspring, on the other hand southward moving cold low salinity Polar and Arctic Waters with signatures from Arctic freshwater sources. We have studied the CO₂ air-sea flux of the relevant water masses in the vicinity of Iceland in all seasons and in different years. We show that the highest ocean CO₂ influx is to the Arctic and Polar

Waters which are CO₂ undersaturated in all seasons. The Atlantic Water is a weak or neutral sink, near CO₂ saturation. These characteristics of the three water masses are confirmed by data from observations covering 30 years. We point out that that future trends in the North Atlantic CO₂ sink are connected to developments in the rapidly warming and changing Arctic.

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Fyrirlestur / Oral presentation 2

E-fuels: past, present and future

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ABSTRACT

E-fuels are liquid and gaseous energy carriers where the primary source of energy derives from electrical energy. Their role as scalable alternatives for the replacement of conventional fossil fuel has become increasingly relevant as means to reduce GHG emissions and local air pollution from heavy transport, marine and aviation. Carbon Recycling International has for the past 16 years pioneered the process development and scale-up of a direct CO₂ hydrogenation process¹ to produce methanol. This process was first demonstrated at the George Olah² Renewable Methanol plant in Svartsengi, Iceland. The company is now commissioning the first large-scale CO₂-to-Methanol project in Anyang, China having the capacity to produce 100.000 tons per annum of methanol. The talk will present a brief history of e-fuel developments in Iceland, its current status and present future scenarios for an energy transition in Iceland based on the domestic production of e-fuels.



Figure 1. 3D conceptual rendering of a 100.000 t/y e-methanol plant under development

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The decade of hydrogen: where are we heading to?

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²Grein Research ehf., Dunhagi 5, 107 Reykjavík, Iceland

ABSTRACT

Global climate change is a scientifically well-recognized phenomenon and appears to be accelerated due to greenhouse gas (GHG) emissions such as carbon dioxide or equivalents (CO_{2eq}). Energy production remains a large factor in GHG emissions, contributing about ~25% of GHG emissions in 2010. To avoid more CO₂ emissions, methods such as electrolytic-produced hydrogen through water splitting, becomes a promising alternative as an environmental-friendly fuel. Yet, the scarcity of freshwater, makes some processes unsustainable, and the aim is to find sustainable ways to produce hydrogen from, for example, seawater, which can be used in many processes such as fuel cells, or ammonia production. In this seminar, we will briefly discuss the underlying problems that come along when producing hydrogen using seawater and how we can optimize the existing methods. Then we will illustrate how theoretical and chemometrical studies through Bayesian Machine Learning can be implemented to combine diverse inputs like empirical data, welfare analysis and market-driven analyses to achieve insight into the socio-economic effects of introducing hydrogen as a clean energy carrier. Finally, this leads to reflections on the question: How can we make optimal investment into hydrogen production?

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2. Fan, L. *et al.* Strategies in catalysts and electrolyzer design for electrochemical CO₂ reduction toward C2+ products. *Sci. Adv.* 6, 1–18 (2020).
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FeSi production in Iceland – Environmental impact and how to improve

Steinar Birgisson¹

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ABSTRACT

Elkem Iceland is a production facility within Elkem ASA that has been producing 65-75% ferrosilicon (FeSi) both in standard (STD) and high purity (HP) grade since 1979 (1). FeSi is a metal alloy that is highly important in the production of steel and cast iron. It plays a role in removing oxygen and oxides from steel and/or acts as an alloying agent. HP FeSi is for example important in the production of electrical steel used for example in electrical generators and electrical motors. HP FeSi is therefore an important part in producing windmills and electrical cars helping us to a greener tomorrow (2).

The presentation will introduce the chemical/industrial production process of FeSi and its environmental impact. Furthermore, it discusses ways to mitigate the environmental impact that have been implemented at Elkem Iceland and other FeSi production plants. Special emphasis will be on the carbon dioxide (CO₂) life cycle analysis (LCA) of the finished FeSi product as a tool for quantifying the specific CO₂ emission for specific products and to identify possible mitigation strategies.



Figure 1. FeSi metal

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Wheat bran-based biorefinery: Extracting bran components through fractionation based on steam explosion and hydrotropic extraction

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¹Division of Biotechnology, Department of Chemistry, Faculty of Engineering, Lund University, SE-22100 Lund, Sweden

ABSTRACT

There is an urgent need in the chemical industry to harness sustainable resources to replace our dependence to fossil fuels. Wheat bran, one of the main by-products of the wheat processing industry, can serve as an alternative feedstock for chemical production because of its valuable structural components including starch, cellulose, hemicellulose, lignin and protein. The challenge for unlocking wheat bran's potential in biomass utilisation is to efficiently fractionate its components. Multiple stage fractionation methods involving steam explosion and hydrotropic extraction were investigated in the present research, The aim was to release the main structural components of wheat bran in a series of separate streams, for facilitating further valorisation. Starch treatment involving industrial amylases and amyloglucosidases effectively solubilises glucose from the starch portion of the biomass. Alkali hydrolysis releases the protein from the de-starched biomass. Steam explosion efficiently releases the hemicelluloses. Hydrotropic extraction using sodium xylene sulfonate solubilised lignin, which was then easily precipitated. And finally, cellulase treatment of the sequentially treated bran improved significantly compared to non-sequentially treated bran. The work presented a promising approach for fractionation of wheat bran. Further work is thus encouraged for valorisation studies of the component streams.

Brush polymers with cyclic and/or divalent side chains

Luis A. Arana¹, Gunnhildur D. Gunnarsdóttir¹, Sigurður G. Gunnarsson¹ and Benjamín Ragnar Sveinbjörnsson¹

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ABSTRACT

In this project, various synthesis of cyclic^{1,2} (A) / linear^{3,4} (B) random, controlled and block bottlebrush copolymers (BBCPs) (**Fig. 1**) containing different cyclic macromonomers (MMs) have been synthesized through Ring Opening Metathesis Polymerization (ROMP). A Chain Transfer Agent containing a thiolactone group (TLA-CTA) has been synthesized to perform Reversible addition–fragmentation chain-transfer polymerization (RAFT) to obtain linear-cyclic MMs through disulphide bridges redox reactions⁵. Conveniently, an *exo*-himic imide containing a primary amine was used to open the thiolactone group in the polymer to obtain the desired disulphide system⁵ and at the same time to perform a ROMP reaction, obtaining the desired BBCPs. Different monomers as Styrene, Acrylonitrile, Methyl Methacrylate, Butyl Methacrylate and Methacrylic Acid have been used in the RAFT polymerization, providing different MMs to obtain diverse optical and mechanical properties to the final BBCP. Kinetics of homopolymerizations for different MMs were measured. A study for controlling the opening/closing of the cyclic/linear side chains through disulphide bridges redox reactions for the different brush copolymers and homopolymers is also being performed. The effects of oxidizing thiol groups in different concentrations, and the possibilities of inter- and intramolecular rearrangements of the disulphide bonds is also being studied.

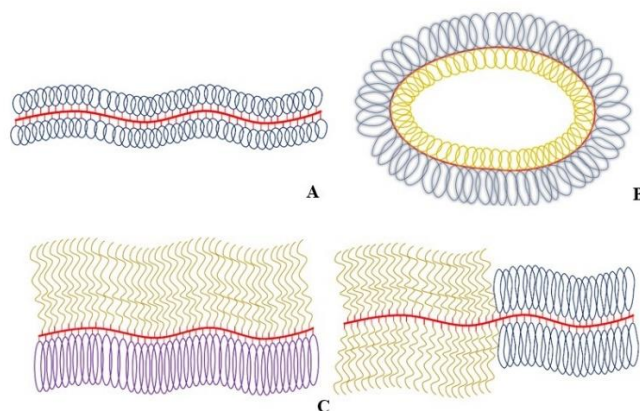


Figure 1. Examples of linear bottlebrush copolymers with homogeneous (A) heterogeneous (B) cyclic MMs and heterogeneous (C) block copolymer (D) Linear Macromonomers.

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1. Milner, S. T. *Science*, **1991**, 251 (February), 905.
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Are transition metal nitrides suitable electrocatalysts towards the nitrogen reduction reaction?

Fatemeh Hanifpour^{1,2}, Camila P. Canales¹, Emil G. Fridriksson³, Arnar Sveinbjörnsson², Tryggvi K. Tryggvason³, Jian Yang¹, Connel Arthur¹, Sigríður Jónsdóttir¹, Anna L. Garden⁴, Sveinn Ólafsson¹, Kristján Leósson⁵, Líney Árnadóttir⁶, Erik Lewin⁷, Younes Abghoui¹, Árni S. Ingason³, Fridrik Magnus^{1,3}, Helga D. Flosadóttir^{2,8}, and Egill Skúlason^{1,2,8}

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ABSTRACT

Electrochemical reduction of dinitrogen to ammonia at ambient conditions is investigated in a three-electrode setup, two-compartment micro-reactor flow-cell using thin film surfaces of polycrystalline VN, CrN, NbN, and ZrN. Electrochemical techniques are used to characterize the surfaces and study the favourable nitrogen reduction reaction and the competing hydrogen evolution reaction. Chronoamperometry loops are used for ammonia production analysis. Accurate and automated quantification of ammonia with a limit of detection of 1 ppb is accomplished in a flow injection analyzer in-line with the micro-reactor. The results show the effect of presence/absence of N₂(g) within both the electrochemical characterization and ammonia production for ZrN. However, no ammonia is detected from studies on CrN in N₂(g) medium. VN and NbN are inactivated upon reacting their inherent N atoms of the surface top layer(s). The overall analyses of the results obtained from ammonia measurements, electrochemical impedance spectroscopy analysis, surface stability checks during the experiments, and surface characterization after the experiments using X-ray reflectivity, reveal certain trends indicating catalytic behaviour for ZrN. However, the concentration of produced ammonia is below the limit of detection of the methods devised to analyse the samples from isotope labelling experiments. The onset of ammonia production on ZrN appears to be in close agreement with that predicted previously by computational studies.

Screening of transition metal nitrides as electrocatalysts for nitrogen reduction using operando ammonia quantification

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ABSTRACT

Ammonia (NH₃) is one of the most widely produced chemical in the world, mainly used for fertilizer ensuring global food security, and is increasingly being recognized as a future sustainable and energy-dense fuel. [1] Electrochemical synthesis is an attractive solution to produce ammonia in a sustainable pathway: reducing nitrogen (N₂) to ammonia through the reaction: $N_2 + 3H_2O \rightarrow 2NH_3 + \frac{3}{2}O_2$. However, this reaction suffers from the low selectivity due to the inherent inactivity of N₂ and to the competing hydrogen evolution reaction (HER): $2H^+ + 2e^- \rightarrow H_2(g)$.

Theoretical work has predicted transition metal nitrides (TMNs) as promising catalytic materials towards the nitrogen reduction reaction (NRR). [2] However, recent experimental studies have shown release of lattice nitride to ammonia in a noncatalytic process for both vanadium and niobium-based nitrides, suggesting inherent instability of these materials. [3-5] Here, niobium-based TMNs are studied further with the aim to increase their stability by systematically changing chemical composition and maximising access to nitrogen using gas diffusion electrodes. Operando ammonia quantification is carried out using an in-line sequential injection analyzer (SIA), where all produced ammonia is reacted to form a fluorescent compound detected in a photomultiplier tube. The technique is automated with detection at the ppb level, allowing for time-resolved measurements synchronized with the electrochemistry. [6]

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Exploring the prevalence of weak allosteric effectors in non-allosteric metabolic enzymes

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ABSTRACT

Protein allostery is an intriguing regulatory phenomenon that has been given various definitions in the literature over the decades, with the latest suggesting that all dynamic proteins have the potential to behave allosterically under certain circumstances. The interactions involved in allostery can range from weak ($K_d = \mu\text{M-mM}$) to strong ($K_d = \text{nM-pM}$). In this study, we intended to examine the prevalence of (weak) allosteric interactions in enzymes that have been classically defined as non-allosteric. As proof of principle, we performed binding assays on several non-allosteric enzymes in the glycolytic pathway with natural metabolites from a customized compound library. Here we used the Microscale Thermophoresis (MST) as a screening method which is capable of detecting binding events in the mM range. Having identified potential binders ($K_d \leq 15 \text{ mM}$), we next proceeded to assess the effect of these binders on the enzymes' activity using enzyme assays. A few potential hits appeared to have weak inhibitory effects on the enzymes, leading to a partial decrease in their activity, and two of the metabolites exhibited non-competitive mode of inhibition, possibly due to binding to an allosteric site. Furthermore, the effect of the ligands on glycolytic- and mitochondrial activities was tested using an in vitro cell assay (SeaHorse XFe96). Additionally, to examine how these ligands affect protein stability, we monitored their interaction with the enzymes using thermal shift assays. The task ahead will be to reveal their binding sites using X-ray crystallography. All the hits we have identified so far are relatively weak binders, with K_d in the range of 6-15 mM, thus we are hoping to expand the compound library to evaluate how extensive weak metabolite regulation is in metabolic pathways and reveal its significance in maintaining cell homeostasis.

* The authors marked with an asterisk equally contributed to the work

Synthesis of chitosan derivatives and structure-antimicrobial activity

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ABSTRACT

Chitosan is a biocompatible biopolymer used in regenerative medicine applications, in drug delivery, and as an antimicrobial substance. Much work has also been devoted to the chemical modification of chitosan to introduce substituents on the 2-NH₂ amino group and the two 3-O and 6-O hydroxyl groups in the β -4 linked glucosamine monomers forming the polymer. The aim has been to improve bioactivity and physicochemical properties.

We have developed TBDMS protection strategy for the synthesis of chitosan derivatives to allow chemoselective modification of the amino group of chitosan and precise control of the degree of substitution [1-3]. This has been combined with a detailed NMR analysis to confirm the chemical structure and determine DS. The activity has been measured against bacteria with a broth-microdilution assay. The resulting MIC values and structural information have been used to construct structure-activity relationships for chitosan derivatives. These studies have shown a strong correlation between the degree of quaternization of the ammonium groups and the antibacterial activity [4]. In contrast, there is a negative correlation between the activity and the length of a spacer group separating the cationic group from the polymer backbone [5, 6]. The antibacterial activity of N, N – dimethyl, N - alkyl, and N – methyl, N,N- dialkyl chitosan derivatives is highly dependent on the length of the alkyl chain [7]. Still, the relationship depends on the bacterium species. Antibacterial activity correlates with DS for N,N,N - trimethyl groups, whereas there is no correlation with the DS for the 2-hydroxypropyl-3-N,N,N trimethylammonium groups, and the DS for the 2-hydroxypropyl group in HP chitosan correlates with a reduction in activity [8, 9]. N,O – Carboxymethyl derivatives are inactive against bacteria [9]. The activity of highly substituted N,N,N-trimethyl chitosan against *S. aureus* increases with molecular weight (Mw) up to Mw around 50 Kd, defined as critical molecular weight for activity (CMW), after which the antibacterial effect is independent of Mw[10].

In future studies, the group is planning to leverage the understanding of the structure-activity relationship in applications, including wound treatment, coatings, and nanoparticles based on chitosan derivatives.

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Crystal habit modification of metronidazole by supramolecular gels with complementary functionality

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ABSTRACT

Supramolecular gels based on low molecular weight gelators (LMWGs)¹ have been used as media for crystal growth² to crystallize inorganic substances, proteins, and active pharmaceutical ingredients due to various advantages, such as facile synthesis, long shelf-life, and easy modification of functional groups.³ The gel-solute interactions influence both nucleation and crystal growth rates in a supramolecular gel phase crystallization.⁴ We have synthesized a series of bis(urea) compounds with complementary functional groups similar to pharmaceutical drug metronidazole (drug mimetic) and its structural isomer isometronidazole (non-mimetic). Metronidazole, a nitroimidazole antibiotic, is used to treat periodontal disease and shows activity against anaerobic protozoa and bacteria.⁵ The drug mimetic and non-mimetic compounds formed gels in various solvent/solvent mixtures. The thermal and mechanical strength of the isomeric gelators was compared using sol-gel transition temperature and rheology and the morphologies of the xerogels were analyzed by scanning electron microscopy (SEM). Crystallization of metronidazole in the drug mimicking gels resulted in a marked habit modification of the metronidazole crystals (Figure 1), which was not observed with the non-mimetic isomeric gels. These results indicate that the drug-mimetic gels interact with the surface of the drug crystal, giving rise to new morphologies. In this talk, the importance and the future scope of supramolecular gel phase crystallization will be discussed.

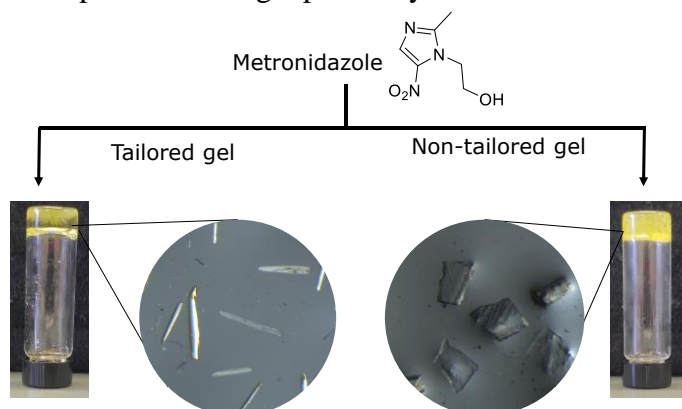


Figure 1. Gel phase crystallization of metronidazole in drug mimetic and non-mimicking gelators.

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Electrocatalysis for Green Production of Hydrogen

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ABSTRACT

Rapid increase in world's food and energy demand due to global development and population surge led to increase in fossil fuels consumption. This heavy dependence on fossil fuels has not only caused their rapid depletion but also attributed to detrimental environmental issues and emergence of global warming. Hence to preserve human societies and the environment but yet enable sustaining long-term development, there is an urgency to develop renewable and clean alternatives for production of high-value-added chemicals and green strategies for energy storage and energy carrier purposes. Coupling renewable sources of energy with electrochemical technologies, if done efficiently, could tackle the non-dispatchable nature of renewables by providing storage in chemical bonds. Hydrogen as a part of renewable energy plays an important role in the construction of clean and sustainable energy system, and electrochemical water splitting to produce hydrogen has been a clean, efficient, and sustainable strategy to replace fossil fuels. However, the relatively high energy consumption on the surface of electrodes makes it difficult in realizing the widespread application. Therefore, the development of high efficiency electrocatalytic systems to reduce the overpotential is essential to promote such industrialization. To realize industrial-scale H₂ production, substantial challenges on both the fundamental (i.e., catalyst activity and selectivity) and system levels (i.e., mass transport, conversion rate, and energy efficiency) need to be addressed. Here the focus is on the fundamental side where platinum, ruthenium and other precious metals still have the highest hydrogen evolution activity in acid and base solution, while their natural scarcity limits their extensive application and thus other catalyst materials need to be explored which are cheap and abundant and at the same time offer activities close to what those metals have. To address this challenge, state-of-the-art Density Functional Theory (DFT) calculations have been used on modelling new class of electrode materials for the possibility of hydrogen evolution reaction. The result was interesting as similar activation energy of H₂ evolution as on Pt and small overpotential of near zero volts to adsorb proton on the surface for initiation of the reaction was found for the studied material which makes it interesting for further experimental investigations¹.

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Veggspjöld
Poster presentations

A Gas-Phase study on the role of low energy electrons in inducing dissociation to a potential gold precursor for FEBID technique

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ABSTRACT

As focused electron-beam induced deposition (FEBID) of metallic structures mainly relies on organometallic precursors, its applicability for writing functional nanostructures, e.g. with well-defined magnetic or conductive properties, is critically dependent on the precursor's decomposition under the electron beam. Preferably such precursors have fairly high vapour pressure, are stable under ambient conditions but decompose completely under the electron beam. Gold precursors for high purity gold deposition in FEBID are precursors that have significant potential in number of applications such as plasmonics and nanoelectronics.¹

Here we present a study on one such precursor; Methylgold(I) trimethyl-phosphine, $(\text{CH}_3)_3\text{AuP}(\text{CH}_3)_3$, and in context to the role of low energy secondary electrons in the deposition process^{2,3}, we have studied dissociative ionization of this precursor under single collision conditions in the gas phase as well as its performance in FEBID under UHV conditions. We have determined the appearance energies for individual fragmentation processes and calculated the respective thresholds at the TPSS/def2-TZVP and DLPNO-CCSD(T)/QZVPP levels of theory to aid the interpretation of the underlying fragmentation processes. Further, ion yield curves were recorded for individual fragments and used to derive the average carbon and phosphor loss per DI incident in comparison to the FEBID deposit composition. The performance of this precursor is evaluated with respect to its stability and volatility and the deposits composition is determined by means of Auger electron spectroscopy.

In a previous FEBID study on this precursor under HV conditions⁴, the deposits fabricated were found to consist of 19-25 at. % Au, 54-62 at. % C, and 2-7 at. % P. We find that the gold content is increased considerably under UHV conditions and that the underlying fragmentation pathways are markedly different. The Methyl-gold(I)-trimethyl-phosphine is a good precursor for production of fairly high gold content deposits because of its handling, stability, and volatility.

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Persistent water-soluble nitroxide biradical for in-cell DNP-NMR

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ABSTRACT

Over the past decade, solid-state dynamic nuclear polarization (DNP) nuclear magnetic resonance (NMR) spectroscopy has been emerged as a powerful technique to unravel the complex biomolecular structures at atomistic resolution. DNP serves to overcome the inherent insensitivity of NMR by the polarization transfer from electrons to surrounding nuclei under microwave irradiation. The sensitivity gain conferred by DNP enables the detection of biomolecules at their physiological concentration. Nitroxide biradicals such as bcTol-M¹ (**figure 1**) have been shown to be excellent polarizing agents for high field DNP. Recent studies involve the use of these biradicals as polarizing agents in mammalian cells². However, the short lifetime of these radicals in cellular environment and low solubility in aqueous solutions limits their *in-cell* applications. Sterically-shielded nitroxide radicals³, such as nitroxides flanked by ethyl groups instead of methyl groups, are stable under reductive conditions. However, they are not soluble in aqueous solutions. Herein, the synthesis and structural characterization of a new sterically shielded and highly water-soluble nitroxide biradical (**1**), a derivative of bcTol-M¹ that was previously synthesized in our group, will be discussed. This biradical will be used for *in-cell* DNP-NMR measurements.

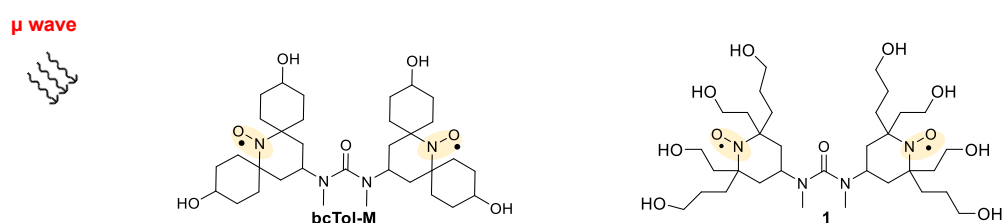


Figure 1. Binitroxide polarizing agents bcTol-M and **1**.

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Slow pyrolysis of nutshells into gaseous, liquid, and solid biofuels

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ABSTRACT

Due to the worldwide energy concerns and fossil fuel depletion as well as environmental problems associated with their use, renewable energy sources are getting increased attention. Biomass has been recognized as one of the alternatives to fossil fuels due to its global availability and environmental benefits. Biomass utilization in traditional combustion processes is however limited due to its low energy density [1] and its contribution to the release of very toxic organic compounds, such as dioxins [2]. However, pyrolysis is a promising thermochemical technique that can be used to thermally degrade biomass into a range of useful products, such as char (solid), bio-oil, and fuel gas products (volatiles) [3].

In this study, a fixed-bed reactor is used to study the effect of condensing temperatures of biomass pyrolysis vapors on bio-oil yields. Given the different methods of vapor condensations, the results obtained in this study are for a dry-ice bath and a bath with a mixture of dry-ice and ethylene glycol (in the latter case the temperature of the bath was reached -60°C). The effect of condensing temperature on bio-oil yields was investigated at condensing temperatures from 100 to 10°C as for the bio-oil capture the temperature of the bio-oil trap should not go above 30°C [4]. Bio-oil yield increases via the reduction of condensing temperature where the condensing efficiency increased from 0.05 to 0.25 with decreasing temperature. According to the experiments, as the temperature is raised, the gas and bio-oil yields increased. Char yields dropped from 37% to 23% with the temperature increase from 300 to 600°C while volatile yields increased from 64% to 77%, respectively.

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Calculating Nuclear Resonance Vibrational Spectra of Iron-Sulfur Clusters with a Quantum Mechanics/Molecular Mechanics Approach

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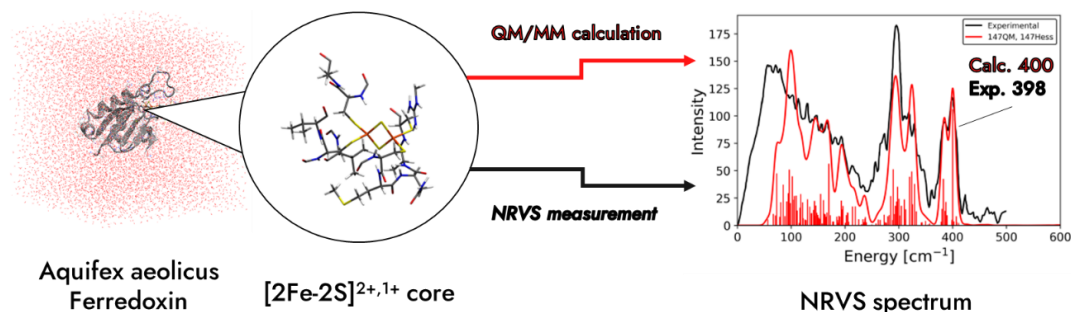
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ABSTRACT

Biological nitrogen fixation is an important part of the global nitrogen cycle where the nitrogenase enzymes catalyse the difficult reaction of dinitrogen to ammonia with the help of complex polynuclear iron-sulfur cofactors.[1] In contrast to industrial nitrogen reduction which takes place at high temperatures and pressure, the nitrogenase enzymes can reduce dinitrogen to ammonia at ambient conditions. If it is possible to understand in molecular details how the nitrogenase enzymes catalyse the reaction, then a bioinspired catalyst may be designed for industrial ammonia production at ambient conditions. However, the reaction mechanism of the nitrogenase enzymes is poorly understood and many details about the reaction mechanism (*e.g.*, the binding site of dinitrogen) are still being debated. Therefore, additional experimental data that can shed light on the structure of reaction intermediates, such as from vibrational spectroscopy, is needed.

Nuclear resonance vibrational spectroscopy (NRVS) is a highly selective vibrational spectroscopy method that yields information only of vibrational modes of a Mössbauer active isotope of an element.[2] It is in particular useful for iron-sulfur proteins as ⁵⁷Fe is a NRVS active nucleus and information of vibrational modes only involving iron can be obtained. It is a promising technique for the study of reaction intermediates of the nitrogenase enzymes that can be isolated. However, owing to the complexity of NRVS spectra for polynuclear iron-sulfur clusters such as the cofactors of the nitrogenase enzymes, theoretical calculations are invaluable to fully understand them.

In order to learn how accurately NRVS spectra can be calculated, we have studied systematically four proteins and three molecular crystal systems with high quality QM/MM models (for Mo/V nitrogenase, we use our previously described models [3,4]). Results indicate that accounting for the chemical environment is crucial for calculated spectra to have explicative power. Furthermore, NRVS is found to be sensitive to overall charge and protonation state of iron-sulfur cofactors.



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Sustainable biobased furanic polyester materials

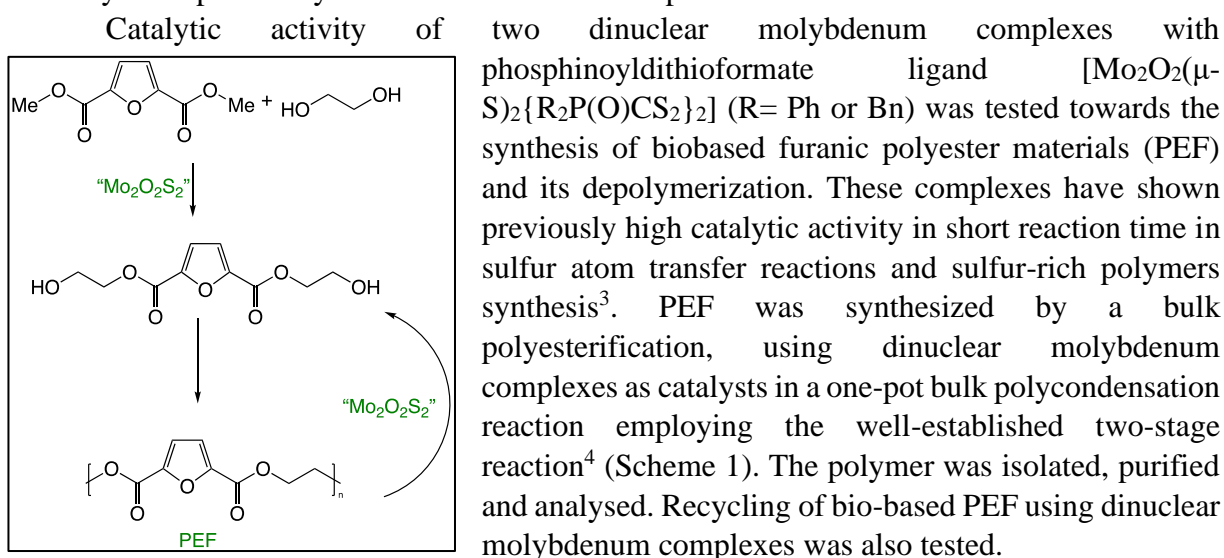
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ABSTRACT

In the last decades, a burgeoning search for sustainable chemicals, polymers, and materials has witnessed the interest in furan-based monomers and the polymers thereof, due to their potential to replace fossil-based counterparts¹. Among the most promising bio-based polymers is indisputably poly(ethylene 2,5-furandicarboxylic acid) (PEF), derived from sugar-enriched biomass. However, very often the use of sustainable approaches for their synthesis is thoroughly overlooked, i.e., mild temperatures, negligible use of solvents, safe catalysts and etc. Also, not so many attempts to recycle bio-based PEF were reported².



Scheme 1. Synthesis and recycling of PEF

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Application of $M^{II}[N_2S_2]$ complexes in Ring Opening Copolymerization

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ABSTRACT

Three different $M^{II}[N_2S_2]$ ($M = Co, Ni$ and Cu) complexes were synthesized and their structure determined. The prepared complexes were screened as catalysts for the ring opening copolymerization (ROCOP) of epoxides and CO_2 , or cyclic anhydrides. The polymers isolated were polyesters and polycarbonates, the conversion was determined using 1H NMR chemical shifts and the relative integrals of the polymers compared to the monomer. The metal complexes were found active for epoxide/cyclic anhydride ROCOP and moderately active for epoxide/ CO_2 ROCOP. The results of the polymerization reactions will be presented showing the catalysts to be a promising class of compounds in ROCOP reactions.

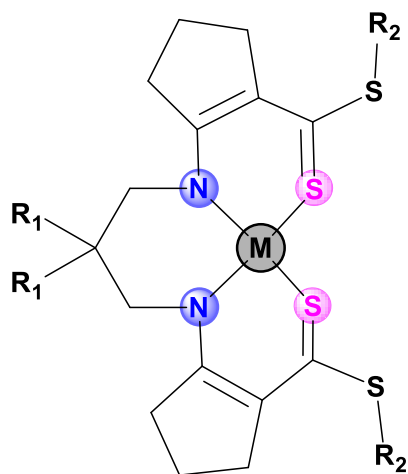


Figure 1. $M^{II}[N_2S_2]$ ($M = Co, Ni, Cu$) coordinated by heterocyclic thioamides ligands

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Spin-labeled RNA to study the Roquin1 1-RNA complex by EPR spectroscopy

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ABSTRACT

Electron paramagnetic resonance (EPR) spectroscopy is valuable technique for the study of structure and dynamics of biomolecules, to obtain information about their functions. It requires incorporation of a paramagnetic center (spin label) into the biomolecule, which can be achieved during chemical synthesis of the biomolecule or post-synthetically.¹ Nanometer distances between the paramagnetic centers can be measured by pulsed dipolar EPR techniques, giving access to biomolecular arrangements and movements. However, the study of biomolecules in their native form has been a challenge, since most EPR experiments are carried out at cryogenic temperatures where the atoms are fixed in a particular conformation. To be able to carry out the measurements at room temperature, we have chosen the large RNA-Roquin1 protein complex, where we plan to doubly label the RNA with a rigid spin label **Çm** (Figure 1),^{2,3} a cytidine derivative that base-pairs with guanine in RNA duplexes. This will allow orientation-selective dipolar EPR measurements on this complex at room temperature.

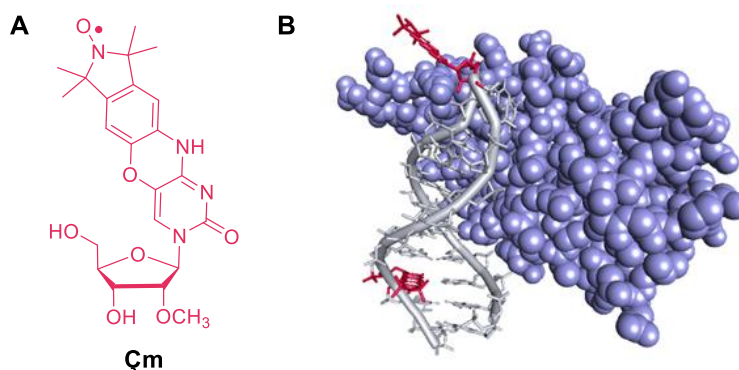


Figure 1. A. Structure of **Çm** spin label. B. X-ray structure of the RNA-Roquin1 complex modelled with two **Çm** spin labels.

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Chiral separation, chromatographic molecular dynamics simulation and spatial distribution of usnic acid enantiomers in lichens

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ABSTRACT

Usnic acid (UA) enantiomers are ubiquitous in a variety of lichen-forming fungi. They are produced in high quantities, and have shown drastically different bioactivities in various bioassays ^{1,2}. Characterising their spatial distribution and enantiomeric ratios in lichens is instrumental to understand their ecological roles and assess their pharmaceutical potential. The study aims to: 1) develop a chiral high performance liquid chromatography (HPLC) method for quantitation of UA enantiomers, 2) elucidate chiral separation mechanisms using molecular dynamics (MD) simulation, 3) assess the spatial distribution of usnic acids in lichen thallus cross sections using Desorption Electrospray Ionization-Imaging Mass Spectrometry (DESI-IMS) and fluorescence microscopy. A chiral HPLC method was developed and validated. MD simulation revealed multiple molecular interactions (e.g. hydrogen bonding) between the stationary phase and analytes driving the chiral separation. Both imaging methods detected UA in the cortex or even surrounding the agal partners. Spatial imaging and chiral HPLC results allow us to infer the predominant usnic acid enantiomer on cross sections. This study highlights the integrative power of imaging analysis and chiral chromatography in understanding the production of natural enantiomers ³.

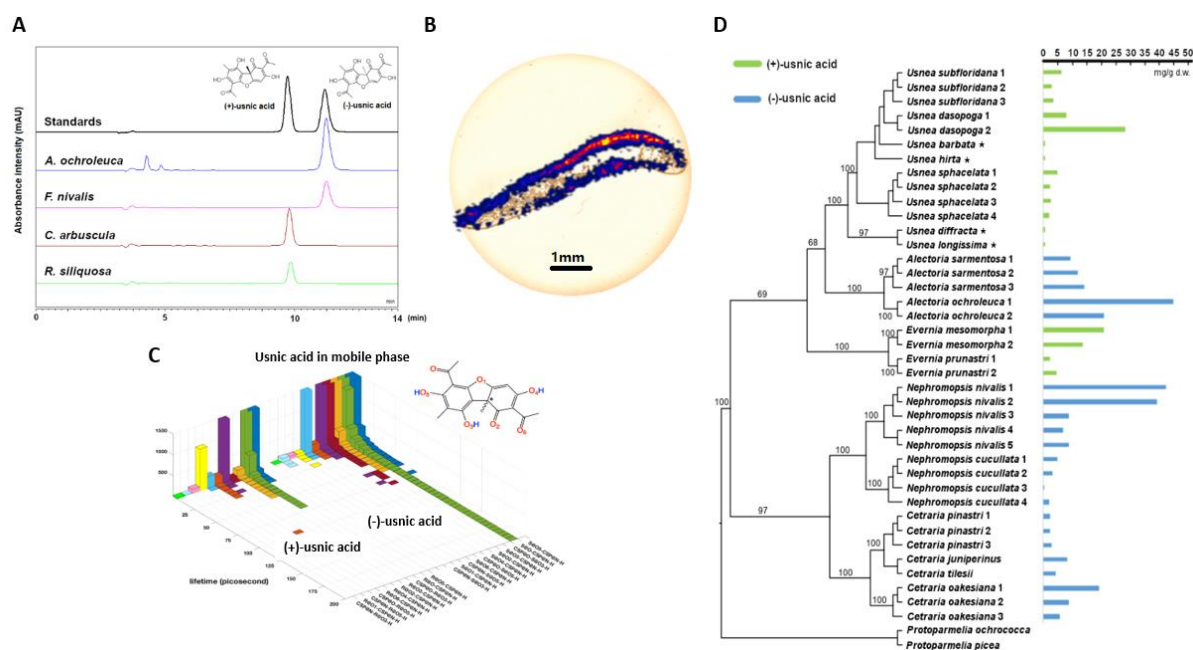


Figure 1. Published and preliminary data about UA enantiomers in lichens. A) chiral separation of UA enantiomers using liquid chromatography, B) imaging mass spectrometry of UA on a thallus cross section (from low intensity in blue to high intensity in orange), C) MD simulation of chiral separation of UA enantiomers, D) phylogenetic pattern of UA enantiomer production.

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Electron beam-induced deposition of Tetrakis(dimethylamino) silane, studied in the gas phase and surface

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ABSTRACT

We studied the reactivity of tetrakis(dimethylamino)silane (TKDMAS) towards low-energy electrons in the gas phase and the composition of its deposits created by Focused Electron Beam Induced Deposition (FEBID). This research was motivated by the use of TKDMAS to produce silicon nitride-based deposits and its potential as a precursor for FEBID. Although there was no evidence of the formation of negative ions by dissociative electron attachment (DEA), there was clear evidence of considerable fragmentation during dissociative ionization (DI). The appearance energies, or AEs, of the fragments generated in DI, were measured. These results are compared to the relevant threshold energies that have been derived using the DFT and linked coupled-cluster (CC) levels of theory. By calculating the average carbon and nitrogen loss per DI incidence, the results are compared to the FEBID deposits left behind by those DI incidents. According to our findings, the DI of TKDMAS is considerably affected by hydrogen transfer processes as well as the development of new bonds. A substantially lower nitro-gen concentration was found in the deposits than was anticipated based on the results of the DI studies. This was an unexpected finding. In addition, the undesirable carbon content of FEBIDs generated from TKDMAS has been removed thanks to the development of a post-treatment technique including the use of water vapour in conjunction with electron exposure. These were also applied to FEBID deposits that were produced with tetraethyl orthosilicate for the sake of comparison (TEOS). On the other hand, the post-treatment of TKDMAS was successful in achieving efficient carbon elimination. The composition of deposits formed using TEOS was only slightly altered as a result of this method.

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Biradicals for selective detection of the binding site in PilA by high-resolution DNP-enhanced NMR spectroscopy

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ABSTRACT

The structural determination of biomolecules at an atomic level is of utmost importance as it unravels functional aspects of the system and is attractive for structure-based drug design. Nuclear magnetic resonance (NMR) spectroscopy provides structural information at atomic resolution under biological conditions. However, the low sensitivity of NMR spectroscopy makes it difficult to study biological samples. In recent years, the drawback has been addressed by dynamic nuclear polarization (DNP),¹ a hyperpolarization technique that involves microwave assisted transfer of spin polarization from radicals (polarizing agent) to nuclei of interest. Here, we will evaluate the postulated receptor-binding site within disulphide-bound loop (D-region) of PilA² using selective DNP (*Sel*-DNP).³ For this purpose, ligand will be functionalised with polarizing agent (**Figure 1A**) and differential spectroscopy (**Figure 1C**) will yield high-resolution multidimensional spectra to specifically highlight residues present in the binding site.

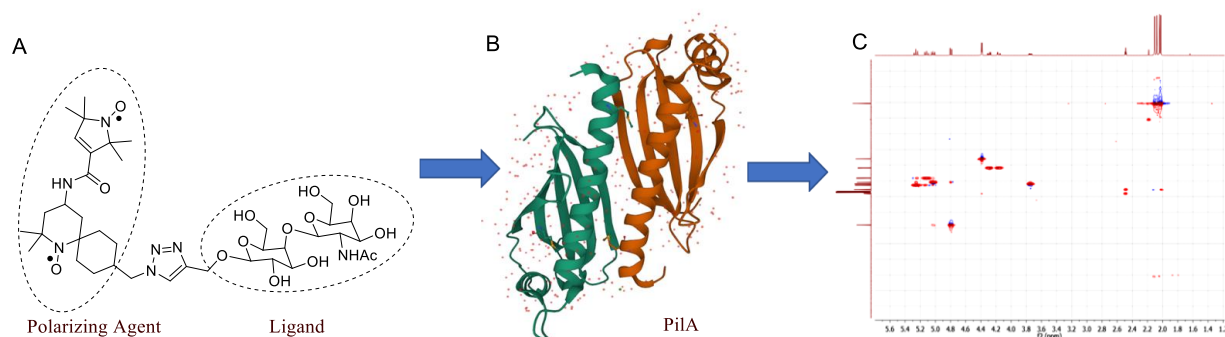


Figure 1. A. Ligand-functionalized polarizing agent. B. X-ray structure of PilA. C. 2D NMR spectrum

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Linear and cyclic brush polymers with cyclic side chains

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ABSTRACT

This project centres around the synthesis of linear and cyclic brush polymers with cyclic sidechains. These polymers will be made using the grafting-through method, where a cyclic macromonomer is first synthesized and then polymerized using ROMP (ring opening metathesis polymerization) and REMP (ring expansion metathesis polymerization) respectively. Many different variations of these brush polymers will be synthesized, such as copolymers containing different types and sizes of macromonomers.

There are two synthetic routes that are being worked on to yield a cyclic macromonomer. Both start off by making a linear macromonomer containing both a terminal alkyne and an azide group which are then coupled together using “click chemistry” to form the ring. The former synthetic route is based on a paper by Jeremiah Johnson’s group at MIT¹, but the second route is an improvement of the synthetic route proposed in Mr. Gunnarsson’s Bachelors project². As said before a key step in both synthetic routes is the ring closing step. A CuAAC reaction (copper(I)-catalysed azide-alkyne cycloaddition) will be utilized in this step, which can be seen in figure 1.

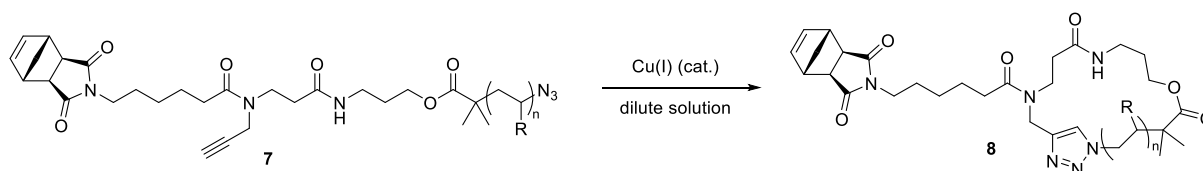


Figure 1: Ring closure of the macromonomer in the first synthetic route

These types of polymers are of much interest since they have a structural motif that has not been analysed in bottlebrush polymers before. Brush polymers have shown many interesting properties. For instance, some brush polymers have shown photonic crystal properties³ and some show potential in drug delivery⁴. Cyclic polymers show better drug loading capabilities than their linear counterparts^{5,6}. Furthermore, brush polymers are better than linear polymers when it comes to drug loading. It will be interesting to see what effect cyclic side chains have on drug loading of brush polymers⁴.

Bottlebrush block copolymers are also known to self-assemble due to their high molecular weight which makes them unlikely to untangle⁴. We theorize that cyclic side chains will make these polymers self-assemble rapidly due to their low chance of entanglement.

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Optimization and structure activity relationship of chitosan-hydroxycinnamic acid conjugates

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ABSTRACT

Chitosan possesses antimicrobial, antitumor, hemostatic, analgesic, film-forming and mucoadhesive activities and is non-toxic, biodegradable, and biocompatible. However, good antimicrobial activity is only achieved under pH 6.5 and chitosan has poor aqueous solubility above this. Chemical modification can be used to overcome these issues.

A new synthesis procedure was developed and optimized by the Design of Experiments (DoE) approach for conjugating hydroxycinnamic acids (HCA-s) to chitosan. Cinnamic acid and *tert*-butyldimethylsilyl (TBDMS) protected HCA-s were converted to their corresponding acyl chlorides and reacted with 3,6-di-TBDMS-chitosan to selectively form amide linkages. Nineteen conjugates were obtained with degrees of substitution (DS) ranging between 3% and 60%. The conjugates possessed improved aqueous solubility compared to unmodified chitosan and were found to be bactericidal against *Staphylococcus aureus* and *Escherichia coli*. The antibacterial activities were equal to chitosan at low DS, however, an increase in the DS correlated with reduced activity. The EC₅₀ values were determined using DPPH (2,2-diphenyl-1-picrylhydrazyl) scavenging assay. While unmodified chitosan only exhibited low antioxidant activity, the HCA-chitosan conjugates enhanced antioxidant activities, correlating with the DS. One caffeic acid conjugate (DS=21%) was found 4000 times more active than chitosan and more active than free caffeic acid.

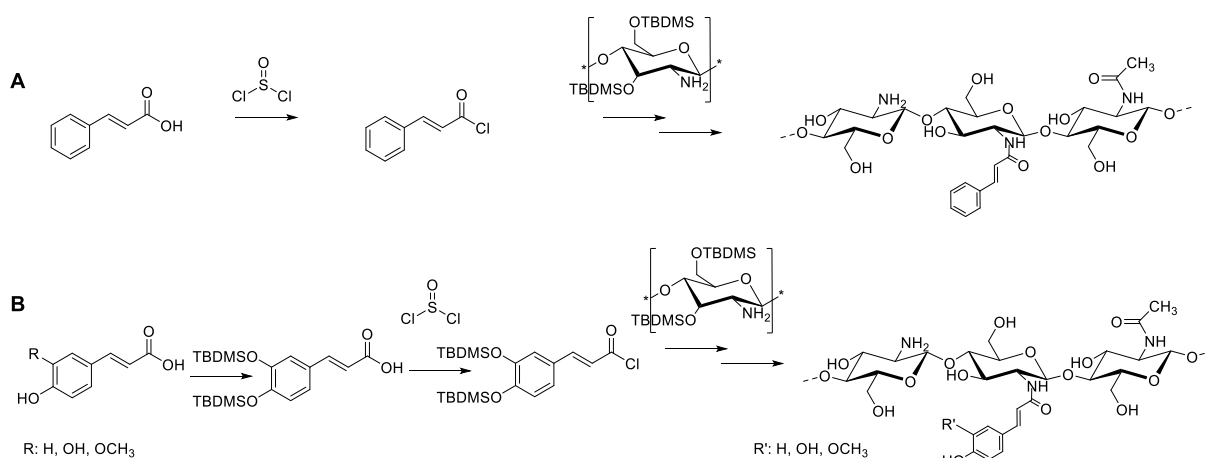


Figure 1. Synthesis schemes for the cinnamic acid-chitosan (A) and hydroxycinnamic acid-chitosan (B) conjugates.

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Exploring the prevalence of weak allosteric effectors in non-allosteric metabolic enzymes

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ABSTRACT

Protein allostery is an intriguing regulatory phenomenon that has been given various definitions in the literature over the decades, with the latest suggesting that all dynamic proteins have the potential to behave allosterically under certain circumstances. The interactions involved in allostery can range from weak ($K_d = \mu\text{M-mM}$) to strong ($K_d = \text{nM-pM}$). In this study, we intended to examine the prevalence of (weak) allosteric interactions in enzymes that have been classically defined as non-allosteric. As proof of principle, we performed binding assays on several non-allosteric enzymes in the glycolytic pathway with natural metabolites from a customized compound library. Here we used the Microscale Thermophoresis (MST) as a screening method which is capable of detecting binding events in the mM range. Having identified potential binders ($K_d \leq 15 \text{ mM}$), we next proceeded to assess the effect of these binders on the enzymes' activity using enzyme assays. A few potential hits appeared to have weak inhibitory effects on the enzymes, leading to a partial decrease in their activity, and two of the metabolites exhibited non-competitive mode of inhibition, possibly due to binding to an allosteric site. Furthermore, the effect of the ligands on glycolytic- and mitochondrial activities was tested using an in vitro cell assay (SeaHorse XFe96). Additionally, to examine how these ligands affect protein stability, we monitored their interaction with the enzymes using thermal shift assays. The task ahead will be to reveal their binding sites using X-ray crystallography. All the hits we have identified so far are relatively weak binders, with K_d in the range of 6-15 mM, thus we are hoping to expand the compound library to evaluate how extensive weak metabolite regulation is in metabolic pathways and reveal its significance in maintaining cell homeostasis.

* The authors marked with an asterisk equally contributed to the work

Þakkir / Thanks

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