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Structure-guided investigation of parameters determining enzyme-catalyzed reactions

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Enzymes play an indispensable role in all molecular processes in life. Their substrate and regio-specificity are embedded in their three-dimensional structure. In addition, the structure also contains information on the biochemical reaction to be performed on the substrate. Thus, knowing the three-dimensional structure paves the way to a deeper understanding of enzyme properties. Equally important are kinetic and thermodynamic parameters in the study of enzyme reaction mechanisms. Therefore, in our research, we integrate these different aspects of enzymology to better understand enzyme reaction mechanisms in order to make enzymes amenable to biocatalysis and drug discovery. Toward these aims, we employ a multidisciplinary approach encompassing kinetic, thermodynamic, spectroscopic, and structural techniques (Figure 1).

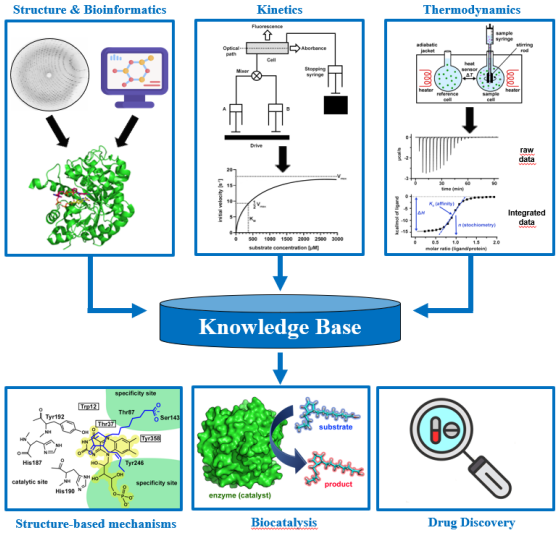

Figure 1: Scheme of our research approach.

Envisaged internal collaborations

Our institute will collaborate with the Institute of Organic Chemistry (Breinbauer group), which will synthesize substrates, coenzyme analogs, and inhibitors. These compounds are needed to shed light on enzyme-catalyzed mechanisms and to develop potential drug candidates targeting specific enzymes.

Furthermore, we will collaborate with the Institute of Molecular Biotechnology (Kourist Group) to assess the potential of enzymes as valuable biocatalysts. For this purpose, we will kinetically characterize promising biocatalysts, providing information about their activity and substrate and reaction scope.

Hot-spots of Microbiome Innovation: AI strategies for the discovery of Microbe-Mediated Environmental Contaminant Remediation

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The principle of microbial infallibility states that microorganisms can evolve to metabolize any organic compound. This principle remains prevalent in bioremediation and raises the question of whether microorganisms can effectively clean up human-made chemical pollutants (O'Malley & Walsh, 2021). Environmental microbiomes exhibit significant metabolic versatility and adaptive potential in response to chemical disturbances. However, it is unknown whether they can degrade synthetic chemicals lacking natural analogs such as the so-called "forever chemicals". Several mechanisms for microbial degradation of such compounds are known, including enzymatic reductive dehalogenation (Wackett & Robinson, 2020). These findings indicate that diverse microbiomes likely contain yet undiscovered enzymatic functionality. Within the frame of the DigiBioTech project - a lead project of Graz University of Technology – we aim to identify new enzymes that facilitate the breakdown of persistent organic pollutants such as PFAS. Our multidisciplinary team combines expertise in biotechnology, data science, and artificial intelligence to address the challenge of finding such rare functions in natural habitats. We utilize omics methods, including metagenomics, metatranscriptomics, and functional analysis—alongside machine learning techniques to guide experimental research and accelerate the discovery of novel enzymes and their functions. By examining highly diverse microbial communities across different habitats and contaminated sites, we aim to identify key taxa involved in previously uncharacterized biodegradation pathways of emerging and persistent pollutants.

Envisaged internal collaborations

Joint projects will deepen our understanding of the microbiome's role in bioremediation. We will explore additional collaboration opportunities to develop systems that enhance microbial activity for contaminant degradation. This could include designing aerobic and anaerobic bioreactors tailored to specific microbial consortia. Additionally, implementing pilot or full-scale systems can facilitate the investigation of reaction kinetics for the bioremediation process, enabling the development of predictive models. These models can then be employed to optimize system design and performance based on microbial growth rates and degradation pathways to effectively remediate polluted environments.

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Investigating the fibrillation process and the characteristics of nanocellulose obtained through high-pressure homogenization

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Nanocellulose has attracted significant attention due to its outstanding properties, including high mechanical strength, low density, large surface area, and biodegradability. [1] These properties can be significantly influenced by chemical modifications. A promising way to produce nanocellulose is high pressure homogenization (HPH). HPH is a mechanical process that employs pressures up to 1200 bar to break down materials into nanoscale sizes. The process involves pumping the material through a narrow gap, thereby generating intense shear forces. The pressure level and the number of passes can be adjusted. It is possible to continuously produce 20 g dry mass of nanomaterial within hours. The nanocellulose can for instance be used as rheological modifier, for coatings or in 3D bioprinting.

The structure of cellulose varies depending on its source, whether derived from plants, bacteria, or algae. Crystallinity, molecular weight, the arrangement of cellulose microfibrils, and the presence of lignin, hemicellulose, other biopolymers and small molecules influence the nanocellulose production process and the properties of the final products. Hence, it is beneficial to gain further knowledge about defibrillation, and the properties of the products depending on the feedstock, and its pretreatment.

In this poster presentation, the fibrillation process was examined depending on different pressure levels during HPH, using refined Eucalyptus Kraft pulp as a precursor material. The fiber size was analyzed using a microscope and a custom-made program.

Envisaged internal collaborations

This work has benefited from the expertise of the Institute of Bioproducts and Paper Technology (BPTI). Continued collaboration, particularly involving the use of the high-pressure homogenizer, holds strong promise for advancing nanocellulose research.

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Covalent Crosslinking of Alginate by Native Chemical Ligation

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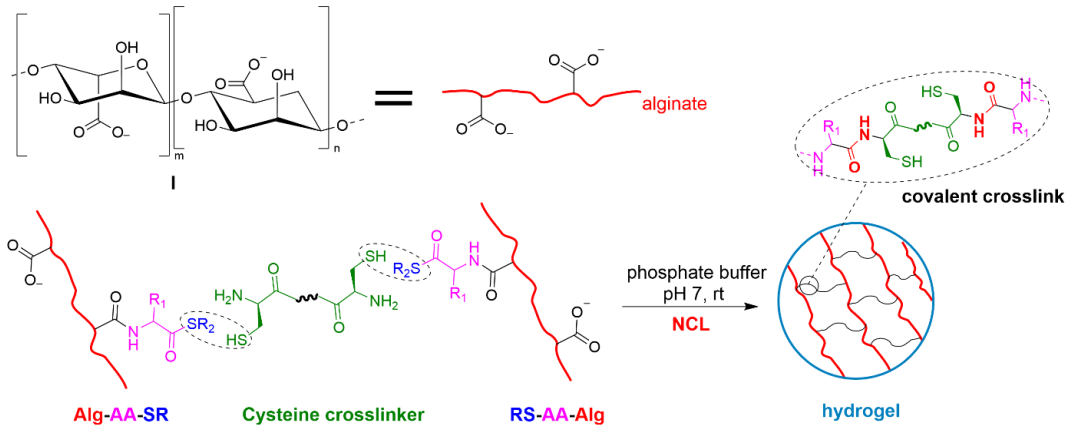
Polysaccharides are often used as polymer precursors for biomedical hydrogel design due to their high natural abundance, renewable character, hydrophilicity, biodegradability and biocompatibility. However, their naturally predefined composition limits their compatibility with many crosslinking chemistries essential for chemical and mechanical stability of produced hydrogels. The resulting need for chemical modification of biopolymers with reactive moieties often hampers their initially favored biocompatibility and motivates a high demand for water-friendly, chemo-selective and non-toxic crosslinking strategies for synthesis of hydrogels with suitable mechanical properties without sacrificing biocompatibility and bioactivity. [1,2]

Native chemical ligation (NCL), a method widely used in protein synthesis, enables covalent bond formation under aqueous conditions without any additional reagents or catalysts, yielding native peptide bonds between C-terminal peptide thioesters and N-terminal peptide L-cysteine residues.[3] In our study, sodium alginate (Alg, I) was functionalized with amino acid-based thioesters (AA-SR) and crosslinked with bifunctional L-cysteine linker molecules. The resulting hydrogels were formed under ambient conditions in an aqueous, pH-neutral medium, offering an innovative approach for covalent crosslinking of alginate compatible with the physiological environment. This method opens up new possibilities for therapeutic hydrogel systems with potential applications in drug delivery, regenerative medicine and tissue engineering.



Envisaged internal collaborations

Biocompatibility / cell viability tests, in vitro cell culture, tissue engineering / drug delivery applications.

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The FSA method: enabling the identification of spectral tuning sites in the red light photoreceptor *Is*PadC

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Phytochromes act as important sensors in many phylogenetic taxa and integrate red and far-red light signals to infer light quality and elicit species appropriate reactions to environmental cues. These light sensing capabilities are governed by amino acids which 1) tune the energetic landscape of the co-factor and 2) stabilize the light-state dependent conformational ensembles of secondary structural elements. The latter are equally important to co-regulate the light-state dependent cofactor conformation and signalling to the effector domains. Historically, research into these light-sensing capabilities focused on residues directly coordinating the cofactor like AspDIP and structural elements like the PHY tongue. However, this view of phytochromes is too simplistic as the highly dynamic nature of these allosterically regulated proteins also allows the involvement of other cofactor distant structural elements in functional fine tuning.

In a recent study, our lab developed an approach which integrates protein sequence design and evolutionary sequence conservation to uncover additional functionally important sites in red-light photoreceptors. In our model protein, the bacteriophytochrome diguanylate cyclase *Is*PadC, this led to the flagging of a beta turn element in the GAF domain. Intriguingly, substituting positions in this turn to remove cofactor distant interactions led to one variant which featured a 10x accelerated thermal reversion rate whereas another showed a more than 10x longer thermal recovery. Thus, this beta turn element, without direct cofactor interaction, could be implicated with tuning of key spectral characteristics in phytochromes. Furthermore, hydrogen-deuterium eXchange mass spectrometry (HDX-MS) experiments uncovered that the beta turn element tunes the conformational dynamics landscape of the phytochrome which is likely causative of the disturbed thermal reversion characteristics upon substitution. These insights expand our understanding of the intricate tuning mechanism which evolved in phytochromes to satisfy specific organismal requirements. Specifically, the observed tuning of conformational dynamics linked to functional properties like thermal reversion might be a research field deserving more attention to further our understanding of phytochrome functions in plants and other light sensing organisms.

Envisaged internal collaborations

This project was recently sucessfully finished as a collaborative effort between the Photobiochemistry and Protein design groups within the Institute of Biochemistry.

Xanthates: Powerful single-source precursors for highly porous metal sulfides

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In heterogeneous (photo)catalysis, the efficiency depends on a plethora of factors, like the absorption coefficent, bandgap alignment, stability and available surface area. Many of these parameters can be tackled by using metal sulfides like $ZnIn_2S_4$[1], $CuInS_2$[2], Cu_3BiS_3[3], $CuSbS_2$, $Cu_{12}Sb_4S_{13}$[4] and $AgBiS_2$[5], showing bandgaps in the lower visible range and high absorption coefficients above 10^5 cm^{-1}. The activity of heterogeneous catalysts however, is limited by the surface area of the catalyst. To address this problem, we synthesized various metal sulfides from the corresponding metal xanthates. These metal xanthates provide both the metal and sulfur source, while reacting to metal sulfide and volatile decomposition products forming micro- or mesopores in the process. The choice of metal and side chain offers control over the solubility, conversion temperature and porosity.[6] Metal sulfides can not only be used as photocatalysts by themselves. They can also be applied as cocatalysts to increase the activity of other photocatalysts, such as the well-known cheap, abundant, and non-toxic photocatalyst titania.[7] We prepared mesoporous titania films and infiltrated them with metal xanthate solutions, which were thermally converted to the metal sulfides. We used the pristine porous sulfides and the sulfides@mp TiO_2 for dye degradation and hydrogen evolution experiments.

Envisaged internal collaborations

The PTC offers a potential valuable insight into the charge transfer of our photocatalysts via oxygen reactive species, which they could track via EPR measurements. The many institutes involved in the Lead Project 03 are a constant source of expertise and techniques, and provide the possibility for many follow-up experiments and projects.

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Alkyne-Functionalized D-*manno*-*C*-Glycosides: Synthetic Hurdles and Unexpected Outcomes

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Urinary tract infections (UTIs), commonly caused by uropathogenic Escherichia coli (UPEC), are triggered when UPEC binds to host cells using fimbriae that contain lectins, such as FimH, which specifically recognize α-D-mannosides. In this context, we previously prepared *O*-glycosidic mannoside derivatives covalently attached to cellulose presenting a polyvalent ligand for FimH.[1] Herein, we present several different approaches for the synthesis of *C*-glycosidic alkyne α-D-mannoside entities. The synthesized compounds will be used for a CLICK-chemistry coupling onto 6-azido-6-deoxy-cellulose[2] and subsequently tested as a polyvalent antagonist against FimH. Synthetic and analytical details will be presented.

Envisaged internal collaborations

For in-depth structural characterization, advanced NMR spectra are measured by Hansjörg Weber from the Institute of Organic Chemistry (TCVB). Intact protein mass spectrometry is performed by Andreas Winkler and Philipp Pelzmann from the Institute of Biochemistry (TCVB) and crystallographic measurements are performed by Roland C. Fischer from the Institute of Inorganic Chemistry (TCVB). Further collaboration is envisioned with the Haas group from the Institute of Inorganic Chemistry (TCVB) and Bernd Nidetzky from the Institute of Biotechnology and Biochemical Engineering (TCVB).

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Deformation and strain measurements at high frequencies using digital image correlation

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Mechanical testing under various loading conditions is crucial for characterizing a material´s properties. It requires an accurate measurement of the sample´s deformation and strain, for example, to determine the fundamental stress–strain curves. Conventional measurement devices typically use strain gauges, differential transformers, or extensometers, which yield only a single point or averaged measurement that is used to represent the macroscopic behaviour of the entire specimen.

Recent advances in digital imaging have enhanced the digital image correlation (DIC) technique, expanding its applicability to capturing 2D and 3D coordinate fields on material surfaces [1]. This method relies on accurately tracking the shifts of a speckle pattern on the sample´s surface by a digital camera. DIC enables the calculation of displacement, strain, strain rate, velocity, and curvature. As a non-contact method, it is unaffected by the material type or the dimensional scale, making it particularly advantageous for analysing complex geometries and heterogeneous materials. Unlike traditional methods, it provides full-field data, offering a more detailed insight into material behaviour. Due to its wide-ranging capabilities, DIC has found extensive applications in various areas such as tensile and fatigue testing, composite material analysis, fracture mechanics, metal forming processes, biomechanics, and high-temperature deformation experiments.

The DIC method is used to measure quasi-static sample deformation, i.e., under slowly changing external stimuli. In this work, we are adapting the use of DIC to measure displacement and strain at high-frequency conditions, particularly those operating at mechanical resonance [2]. For example, piezoceramics are widely used in ultrasonic medical imaging, welding, and precision cleaning. At resonance, displacements typically range from 0.1 to 10 µm at frequencies above 30 kHz. By implementing stroboscopic data collection, we managed to measure the resonance strain behavior of a reference piezoceramic sample at 90 kHz.

Envisaged internal collaborations

Our DIC system can be used to measure deformation, strain, and strain concentrations of polymer, metallic, or ceramic samples of different shapes and sizes from quasi-static to high-frequency conditions, which could reveal basic material properties or critical flaws in material or design. We are also looking for collaborations in the field of FEM simulations of (electro-)mechanical material behaviour.

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Continuous Multiphase Reactions in the Taylor-Couette Disc Contactor

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The development of sustainable process designs in the chemical industry necessitates the implementation of highly optimized reactor concepts. Stirred liquid-liquid extraction columns (Rotating Disc Contactor, Kühni column) at industrial scale are designed to achieve intensive and uniform mixing between two immiscible liquid phases, ensuring efficient mass transfer and process stability. These extraction columns often suffer from insufficient mixing because of dead zones and crud accumulation. The Taylor-Couette Disc Contactor (TCDC) overcomes these disadvantages because of an increased shaft diameter compared to the RDC, rotating discs at the shaft, and the abandonment of the stator discs on the column wall. Because of the rotating discs, the mixing section of the TCDC is segmented into individual compartments, ensuring controlled phase interaction and enhancing mass transfer efficiency. These compartments can be conceptually modeled as a series of continuously stirred tank reactors (CSTRs), arranged vertically to form a compact, space- and equipment-efficient cascade system. In each compartment, two toroidal Taylor-vortices form, which are utilized to retain a dispersed phase in a continuous phase for a defined time. Several continuous processes have been studied in a TCDC DN50, including gas-liquid, liquid-liquid, gas-liquid-solid, and liquid-solid contact. The gas-liquid contact was investigated by neutralizing 0.1 M sodium hydroxide solution with CO_2. Furthermore, a continuously-operated recycling process of lithium and cobalt from lithium-ion batteries was implemented in the TCDC, including the leaching of black mass (shredded cathode and anode material) with carbonated water (gas-liquid-solid, [1]), heterogeneous precipitation of lithium carbonate from alkaline solution with CO_2 (gas-liquid-solid), and the two-step solvent extraction of cobalt with extraction agents (liquid-liquid, [2]). With this process, more than 70% of lithium and cobalt could be recycled from black mass. Another investigated process configuration is the continuous extraction washing of solid particles in the TCDC. This approach is based on the characteristic of the TCDC to act as a cascade of continuous stirred tank reactors, and when applying a counter current flow, serves to provide a high extraction and washing efficiency at a low energy footprint. This application was investigated for the remediation of residues from biogenic glycerol purification [3], and is now undergoing parametric investigation and modelling, as well as being tested on other potential feedstocks.

Envisaged internal collaborations

Ongoing cooperation with BIOTE Institute, also possible cooperation with SOMAP Lab

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Functionalized Hydrosilanes as Next-Generation Precursors for Semiconductor Applications

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The increasing demand for advanced semiconductors in fields such as autonomous systems, cloud computing, and space technologies calls for innovative materials and processing strategies. While single-crystal silicon remains the industry standard, its production is energy-intensive and inefficient. At the **CD-Laboratory for New Semiconductor Materials Based on Functionalized Hydrosilanes**, we explore novel functionalized hydrosilanes and hydrogermanes as liquid, single-source precursors for high-purity silicon films via liquid and vapor phase deposition (LPD/VPD). These compounds decompose cleanly to elemental silicon and enable precise doping (n- or p-type) and band gap engineering.

Our work combines synthetic chemistry with material processing, offering scalable routes to carbon- and oxygen-free silicon layers with tunable electronic properties. The resulting silicon-based materials are evaluated for morphology, conductivity, and optical characteristics, paving the way toward sustainable and flexible semiconductor manufacturing. This interdisciplinary approach, developed within the **CD-Laboratory for New Semiconductor Materials Based on Functionalized Hydrosilanes**, lays the foundation for the next generation of silicon heterostructures in both academic and industrial research.

Envisaged internal collaborations

Collaborations with all institutes of TU Graz interested in semiconductor materials can be envisaged. Especially a collaboration with the FELMI will be necessary for the characterization of the materials.

Fabricate, Degrade, Innovate: Membrane Electrode Assemblies for Polymer Electrolyte Fuel Cells

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Polymer electrolyte fuel cells (PEFCs) are efficient, locally emission-free energy converters that support decarbonization. However, their high production costs and sensitivity to dynamic operation hinder commercialization. Current research aims to improve manufacturing and monitor degradation of the core component, the membrane electrode assembly (MEA). An MEA consists of two electrodes (anode and cathode) on either side of a polymer electrolyte membrane (PEM), with gas diffusion layers (GDLs) added to aid transport of gas, water, and electrons [1].

Research on manufacturing includes a study, which showed that catalyst ink, the basis for electrode manufacturing, can be stored for up to four weeks without subsequent PEFC performance decay [2]. The degradation of MEAs has been investigated in-situ and ex-situ. A method to monitor the state of health of PEMs during accelerated stress tests via fluoride emissions from effluent water by photometric analysis was developed and validated [3]. Investigations on the chemical degradation GDLs showed that Fenton's reagent induces fluorine loss and structural changes that temporarily improve oxygen transport and thus, performance, but eventually impair water management due to increased hydrophilicity [4]. In this context, fluorine-free polyaniline-based coating have been investigated as a promising alternative to conventional hydrophobic GDL treatments [5,6].

The use of half cells for rapid, reliable electrode characterization, isolating electrode degradation via decal transfer, and modelling MEA degradation is within the current scope. This aids to deepen the understanding of PEFC behaviour during operation and support broader adoption.

Envisaged internal collaborations

Future research collaborations are planned with the Institute of Bioproducts and Paper Technology (BPTI) on bio-based membranes and with the Institute of Analytical Chemistry (ACFC) and the Soft Matter Application (SOMAPP) laboratory for analytical ex-situ investigations of developed and degraded materials.

Acknowledgement

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Modification of electrode surfaces for CO_2-capture

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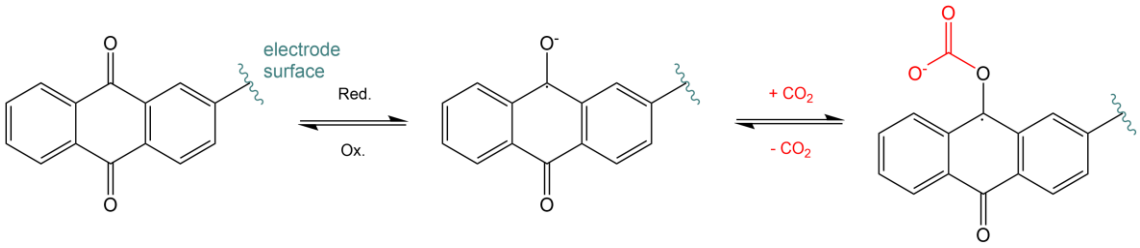
The rapid increase in anthropogenic carbon dioxide (CO_2) emissions to the atmosphere since the industrial revolution is considered one of the greatest challenges of our time. According to the Intergovernmental Panel on Climate Change (IPCC), meeting the criteria of the Paris Agreement on Climate requires not only drastic emission reduction measures, but also the fast implementation of carbon capture utilization and storage (CCUS) technologies. [1]

State-of-the-art technologies are based on the use of diverse amine-solutions, which effectively absorb CO_2 from exhaust gas flows. The captured CO_2 is released and by thermal-/pressure driven desorption. Although so-called amine scrubbing offers a high technological readiness levels (TRL) of 7-9, there are many disadvantages due to the high energy demands for heating and the large physical footprint as well as the involvement of potentially hazardous chemicals. [2, 3]

Electrochemical carbon capture and concentration (eCCC) is a promising alternative to traditional thermochemical processes. Redox-active molecules, such as transition metal complexes, pyridines, dithiols and quinones, have been successfully proven to efficiently and reversibly bind CO_2 (Scheme 1). [3, 4]



Scheme 1: Electrochemical CO_2-capture and release with the example of surface-bound anthraquinone, adapted from [5].

In this work, glassy carbon electrodes were successfully modified with different quinones using chemical and electrochemical grafting methods. These electrodes were then further investigated for their ability to reversibly bind dissolved CO_2 from different electrolytes.

Envisaged internal collaborations

Potential collaborations include the Institute of Organic Chemistry for the synthesis of novel quinones-derivatives and the Institute of Analytical Chemistry and Food Chemistry (ACFC) to conduct GC-measurements.

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Food Packaging in Transition - Ensuring Safety and Quality of Recycled Materials

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Traditional food packaging is undergoing a huge transformation as part of the European Green Deal. The new packaging and packaging waste regulation aims to reduce waste by boosting recycling rates, reusable packaging and renewable materials. Of utmost importance in this respect are the recycled content targets, also for sensitive applications such as food contact. By 2030, single-use plastic beverage bottles and PET packaging must contain at least 30% of post-consumer recycled materials; other plastic packaging, such as polyolefin-based ones, must contain at least 10%. [1] Currently, available polyolefin-based PCR materials lack the required quality and safety to be used as food contact material: in a recent study roughly 1/3 of the tested materials showed genotoxic activity in an Ames MPF test. [2] Furthermore, most of them have an unpleasant off-odour, limiting their suitability and consumer acceptance. Overall, a lack of knowledge on recycling technologies for polyolefins exists. The present work addresses these gaps by combining separation science with toxicological and sensory assessment. Using advanced, hyphenated and multidimensional GC- and LC-based methods, alongside in vitro bioassays, we systematically evaluate the chemical safety, toxicological risk, and sensory quality of polyolefinic PCR materials before and after the recycling process. The poster will provide an overview of contamination profiles found in real-world samples, and demonstrate how linking analytical results with bioassays enables a more robust safety assessment for a sustainable yet safe circular plastics economy.

Envisaged internal collaborations

Collaborations already exist with the Institute of Bioproducts and Paper Technology (BPTI) on safety assessment of fibre-based packaging. More general, our research focuses on the challenges of circular economy, like recycling, reuse, renewable resources, the related quality and safety of products and analytical solutions supporting the transition. The combination of advanced hyphenated and multidimensional chromatographic separation methods with automated sample preparation allows new interdisciplinary initiatives. This newly developed methods are capable of monitoring the sources and formation of undesired components and can be applied to various matrices and purposes (e.g. (waste)water, soil or air analysis; process monitoring and optimization; characterisation of (bio)-products).

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Improving Teraryl based α-Helix Mimetics via Incorporation of *N*-Heterocycles

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The tight net of all our protein-protein interactions (PPIs) has been heavily investigated in the last decades. Their involvement in regulatory processes, makes PPIs attractive targets for academic research and the development of novel therapeutics. [1] Functionalized teraryls have been designed to geometrically mimic the *i*, *i*+4 and *i*+7 amino acid residues of α-helices. [2] Our group developed a modular synthesis of these compounds by sequential coupling of building blocks. After the initially developed scaffold exhibited poor aqueous solubility, this problem was successfully mitigated via the substitution of the outer phenyl rings to 3-pyridyl. However, the solubility of teraryls bearing multiple nonpolar side chains remain problematic. [3-5] This prompted us to investigate the use of *N*-heterocyclic core building blocks within our methodology. The synthesis of multiple building blocks was achieved via a selective Minisici-functionalization of the respective *p*-dichlorodiazines. Sterically guided coupling conditions subsequently allowed for the synthesis of next-generation teraryl based α-helix mimetics with enhanced aqueous solubility.

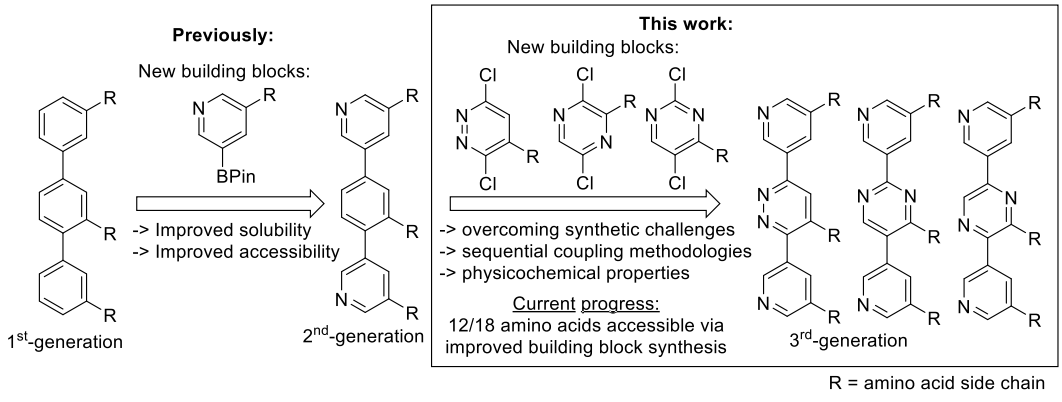

Figure 1: Development of new N-heterocyclic teraryl-based α-helix mimetics

Envisioned internal collaborations

Currently none, as the project is already involved in external collaborations.

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Enzyme Machinery for Bacterial Glucoside Metabolism via a Conserved Non-Hydrolytic Pathway

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In nature, most non-polymeric glucose is found in a chemically bonded form called glucosides[1]. In environments where nutrient availability frequently fluctuates—such as soil and animal gastrointestinal tracts—microbes have developed, alongside hydrolysis, a non-hydrolytic pathway conferred by a single glycoside utilization gene locus (GUL)[2,3]. Compared to the often highly substrate-specific glycosyl hydrolases, the non-hydrolytic pathway offers microbes a chance to use a broader range of substrates by subdividing catalysis into several manageable steps: oxidation and reduction at the C3 position of glucosyl/glucose, eliminative cleavage of the glycosidic bond, and the addition of water.

Building on our study of the phytopathogen *Agrobacterium tumefaciens* GUL[4], we discovered and mechanistically characterized a previously unrecognized, conserved Mn^{2+} metallocenter lyase employed in the hydration step. By extending our search of GUL-encoded lyases, we also identified a Ca^{2+} metallocenter active site in a putative glycoside hydrolase-like protein from *Bacteroides thetaiotaomicron*. We demonstrate its unprecedented dual catalytic function: the eliminative cleavage of 3-keto-glucosides of α-anomeric configuration, and the subsequent addition of water to the resulting 2-hydroxy-3-keto-glycal product, yielding 3-keto-glucose.

Our results reveal a core set of GUL-encoded lyases involved in glucoside metabolism and enable the targeted search for GUL operons across bacterial genomes. Furthermore, we highlight the physiological significance of GUL genetic diversity among bacteria.

Internal collaborations

The ongoing research on *Bacteroides thetaiotaomicron* and the human intestinal bacterium PUE GULs is being conducted in collaboration with Prof. Gustav Oberdorfer for structural analysis and Prof. Pedro Alejandro Sánchez Murcia for quantum mechanics/molecular mechanics (QM/MM) simulations.

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Reactor Design for Azo Dye Synthesis: Transfer of a Two-Step Reaction from Batch to Continuous Flow

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Azo dyes comprise more than 60% of the currently used dyes [1]. They are widely utilized for the photometric analysis of different metal ions in wastewater and medical applications, as well as in the textile and fine chemicals sectors. The production of azo dyes involves forming diazonium salts as a key intermediate. These salts are very reactive, thermally unstable, and can be explosive [2]. Given the risks associated with diazonium salt production and its exothermic nature, it is crucial to manage these substances carefully and maintain precise temperature control.
Flow chemistry minimizes the risks associated with handling diazonium salts by reducing reaction volume, facilitating in situ quenching of intermediates, and enhancing heat transfer [3]. Furthermore, continuous flow systems allow for real-time control of processes, enabling accurate adjustments to reaction parameters such as temperature and pH value.
We introduce a two-step flow setup for the continuous synthesis of an azo dye based on chromotropic acid. In the initial phase, a tubular reactor paired with a 3D-printed static mixer is utilized. An external thermostat regulates the temperature required for the diazotization reaction. During the second phase, the reaction occurs in a 3D-printed continuous stirred tank reactor (CSTR), with a modified design as reported in [4]. The CSTR's jacket allows for precise temperature regulation via an external thermostat, and a magnetic stirrer facilitates stirring. Furthermore, the reactor design incorporates a pH probe positioned at the top of the CSTR to monitor the pH value in real-time. A control loop modifies the base flow rate to maintain optimal reaction conditions, ensuring a pH range of 10.5-11.5.
In summary, integrating advanced process control and 3D printing within continuous flow chemistry facilitates ideal reaction conditions for azo dye synthesis and establishes a foundation for high-throughput production.

Envisaged internal collaborations
None

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Data-Driven Exploration of Self-Assembled Materials

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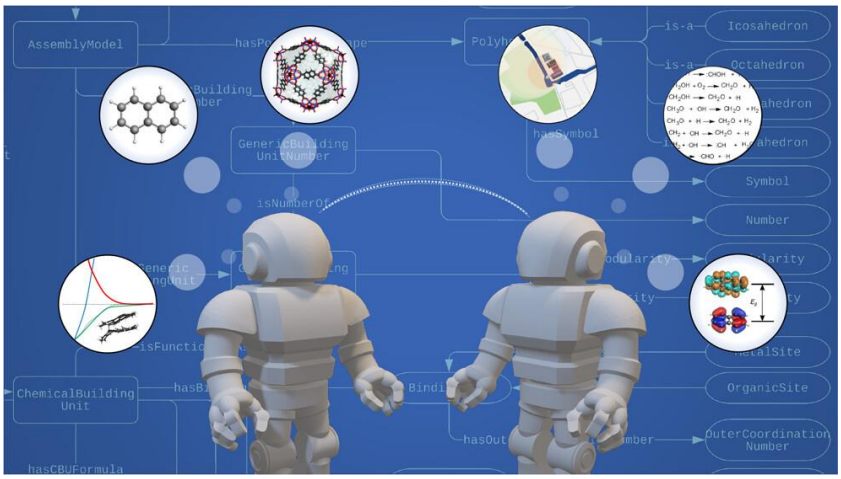
Self-assembly is a cornerstone of materials science, enabling the rational creation of compounds with precisely engineered structures and functions. By translating chemical knowledge into machine-readable formats, we open the door to data-driven strategies in which intelligent algorithms can predict, design, and optimize novel materials and their properties.[1-3] This contribution highlights the current research directions of the Chemical Modelling (CheMin) Group at Graz University of Technology, with particular emphasis on the discovery of inorganic, organic and hybrid (reticular) materials through a synergy of computational modelling, automated data extraction, and machine-learning techniques.[4-6]



Envisaged internal collaborations

Intended to be expanded within the Advanced Materials field of expertise. This includes collaborations on other organic and inorganic material classes within TCVB, and on hybrid organic–inorganic materials encapsulating biomolecular cargo with PTC (TU Graz). In the latter case, artificial intelligence (AI) will be applied to optimize the design and performance of biocomposites (PMWS Lead Project).

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Diarylhalonium-based Probes for Activity-based Protein Profiling of Oxidoreductases

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Activity-based protein profiling (ABPP) represents an intriguing and powerful proteomic method for the *in vitro* and *in vivo* identification and evaluation of proteins in its active state.[1] Throughout all enzyme classes, oxidoreductases (EC 1) have received much less attention, although they play a role in essential metabolic processes and a more detailed insight into their function and activity could be beneficial to the understanding of cellular biochemistry and the role of these enzymes in diseases.[2]

In order to expand the ABPP toolbox for oxidoreductases,[3] we designed and synthesized several novel ABPs for the simultaneous labeling of various subclasses of oxidoreductases based on the potent ALDH2 inhibitor and hypervalent iodine compound diphenyleneiodonium (DPI) and its analogue diphenyliodonium (IDP),[4] making use of their unique reactivity via reductive activation by the target proteins. The probes were then used for *in vitro* ABPP labeling experiments with selected enzymes and fresh mouse liver. After proteome labeling and initial SDS-PAGE in-gel fluorescence assays, promising candidates were further used in biotin/streptavidin affinity enrichment, whereupon labeled proteins could be identified by LC-MS/MS after tryptic digestion.[5]

Envisaged internal collaborations

Further studies regarding the mechanism of action with specific enzymes might be conducted in collaboration with the working groups of Prof. Gescheidt and Prof. Macheroux.

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Next-Level Bioprocessing: CO_2 Utilization by Knallgas Bacteria

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In nature, CO_2 is assimilated into organic compounds by autotrophic organisms, supporting all life forms unable to fix carbon independently. However, anthropogenic activities, particularly large-scale fossil fuel combustion, have led to a 50% rise in atmospheric CO_2 concentrations, disrupting the natural carbon balance. One promising strategy for mitigating this impact and supporting the transition to a sustainable, carbon-neutral bioeconomy is repurposing CO_2 as a feedstock for producing chemicals, materials, animal feed and food. Aerobic hydrogen-oxidizing bacteria (HOBs) are particularly promising, as the high energy yield from hydrogen (H_2) and oxygen (O_2) recombination enables efficient growth on CO_2 as the sole carbon source. An exemplary approach is the lab-scale cultivation of *Cupriavidus necator* on explosive gas mixtures, focusing on CO_2 fixation into polyhydroxybutyrate (PHB) [1]. Achieving efficient delivery of H_2/O_2 mixtures to the cells requires innovative gas transfer technologies to optimize mass transfer into aqueous systems. At Graz, interdisciplinary collaboration between natural and engineering sciences has advanced the technological readiness level of CO_2 fixation by HOBs [2]. Several fermentation facilities were designed, built, and commissioned through partnerships between TU Graz, ACIB, and external safety experts. All systems comply with ATEX regulations and incorporate advanced safety measures, marking a major step toward scalable, safe CO_2-based biotechnological processes [1,2]. Precise controllers enable control of inevitable cultivation parameters and reduce costs using soft sensors. In-depth analysis of media components and gas compositions was pivotal in achieving high cell densities and product contents [3]. This approach opens the unique possibility to engineer and study promising HOBs in tightly controlled chemolithotrophic conditions [4]. New interdisciplinary collaborations between TU Graz, ACIB and industrial partners were initiated and catalyzed the launch of new projects such as the LEAD project ‘DigiBiotech - Digitalisation of Biotechnology’.

Envisaged internal collaborations

New collaborations within the DigiBioTech project have been established with Stefan Radl (IPPT). Further collaborations with CEET and ICTM are planned for product isolation and characterization, respectively.

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Metal-organic frameworks (MOFs) responsive colorimetric sensor for real-time monitoring of food quality

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Biogenic amines produced by food spoilage are an important indicator for assessing the safety of meat and dairy products [1]. Traditional detection methods are difficult to meet the needs of real-time monitoring due to complex operations and expensive equipment.

The Food Responsive Sensor for Colorimetric Observation (FRESCO) project innovatively developed an intelligent colorimetric sensor based on metal organic frameworks (MOFs), which achieves visual detection of biogenic amine concentration through material structure design and response mechanism optimization [2-3]. The sensor exhibits rapid response characteristics in simulated food spoilage conditions and has the potential to be integrated into food packaging materials. By developing low-cost, real-time, colorimetric sensors, it will be possible to monitor the food spoilage status on individual products. The development of sensors that detect specific volatile organic compounds will advance intelligent packaging technology.

Envisaged internal collaborations

We intend to collaborate with the Analytical Chemistry Institute to examine the sensing activity of the developed material (Prof. Borisov) and to assess the potential use for food spoilage monitoring (Prof. Leitner). Additionally, we could collaborate with the Institute of Inorganic Chemistry to examine the crystalline structure under different stimuli (Prof. Amenitsch).

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Size-Controlled enzyme@ZIF Biocomposites: Influence of 1-Methylimidazole on Structure and Function

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Metal-Organic Frameworks (MOFs) are extended porous materials composed of metal ions and organic linkers. Zeolitic imidazolate frameworks (ZIFs), particularly ZIF-8 formed from Zn^{2+} and 2-Methylimidazole (2-HmIm), are commonly synthesized under biocompatible conditions and are suitable for applications such as drug delivery, biosensing and bio-preservation.[1] Our group has shown that biomacromolecules can trigger ZIF crystal growth, forming enzyme@ZIF biocomposites that protect enzymes from harsh environments.[2] We found that synthesis conditions affect the ZIF crystal size and morphology, which directly influence biocatalytic activity. In general, smaller crystals exhibit higher enzymatic activity than their larger counterparts.[3] However, tuning the crystal size by following specific biomimetic mineralization protocols is challenging, thereby limiting control over material properties. In order to address this issue, 1-Methylimidazole (1-HmIm) was introduced as a modulator during the synthesis, with the result that smaller particle formation was enabled, and structural defects were introduced.[4] We hypothesize that these changes would affect the morphology, composition, and catalytic performance of the biocomposites. To test this hypothesis, the effects of varying ligand-to-metal ratios and different percentages of 1-HMiM in the synthesis of enzyme@ZIF systems were examined, using Bovine Serum Albumin (BSA) as a model protein. The resulting BSA@ZIF particles were then evaluated in terms of composition, topology, encapsulation efficiency, and formation kinetics. Furthermore, to investigate the correlation between particle size and enzymatic activity, the synthesis of horseradish peroxidase (HRP@ZIF) biocomposites was conducted. The present study demonstrates that synthesis parameters play a pivotal role in customising enzyme@ZIF biocomposites for particular bio-applications.

Envisaged internal collaborations

We plan to collaborate with the Analytical Chemistry Department at the TU Graz and the Institute of Molecular Biosciences at KFU for optical imaging. Additionally, we see valuable opportunities for joint research with the Institute of Biotechnology at both the KFU and the TU Graz.

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Stereoselective Ring Contractions in Glycopyranosides as Key Step *en route* to Isoiminosugars

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Isoiminosugars are prominent selective inhibitors of glycoside hydrolases, mimicking naturally occurring, carbon chain branched carbohydrates. [1] However, due to their structural characteristics, the synthesis remains challenging. [2] We focus on a $LiAlH_4$ triggered 1,2-shift of C-4 to C-2 in O-2 tosylated glycopyranosides. This stereoselective ring contraction represents the key step on the path to a wide range of isoiminosugars such as 4-*epi*-isofagomine [3] and derivatives thereof. Synthetic details will be presented.

Envisaged internal collaborations

For in-depth structural characterization, advanced NMR spectra are measured by Hansjörg Weber from the Institute of Organic Chemistry (TCVB). Intact protein mass spectrometry is performed by Andreas Winkler and Philipp Pelzmann from the Institute of Biochemistry (TCVB) and crystallographic measurements are performed by Roland C. Fischer from the Institute of Inorganic Chemistry (TCVB). Further collaboration is envisioned with the Haas group from the Institute of Inorganic Chemistry (TCVB) and Bernd Nidetzky from the Institute of Biotechnology and Biochemical Engineering (TCVB).

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Optical biosensors enabling glucose and lactate monitoring in microphysiological systems

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Monitoring glucose and lactate gives valuable information on the viability and the metabolic state of the cultured cells and tissues in microphysiological systems. The production of lactate rapidly increases in the case of mitochondrial dysfunction, for example. Moreover, changes in the glucose consumption rate can be a sign of forthcoming cell death. The majority of available glucose and lactate biosensors are electrochemical [1]. The few reported optical sensors are based on luminescence oxygen-quenching after enzymatic oxidation of the analyte. Despite many advantages of this approach, integration of those sensors into microphysiological systems still remains a challenge.

Previously, we presented an enzyme-based optical glucose sensor that can be straightforwardly incorporated into Organ-on-Chip [2]. In this work, we conducted further characterization of the sensor. Moreover, we adapted the same sensing concept to develop a phosphorescent biosensor for lactate. The sensor consists of oxygen sensitive particles and an enzyme immobilized in a polymeric matrix. To limit the loss of enzyme activity, a catalyst for the decomposition of hydrogen peroxide is added. Sensors are easily integrated by spotting the formulation onto a sealing tape or directly into the microfluidic chip. The spot size can be altered according to the width of the microfluidic channel. Additionally, the dynamic range of the sensor can be modified by implementing diffusion membranes of different porosities.

We evaluated the influence of different conditions (e.g. pH, temperature, spot size) on the sensors' performance, along with the investigation of sensors' stability. Finally, we successfully measured glucose and lactate level in effluent cell culture media from a Liver-on-Chip system. The results were compared to a commercially available method.

Envisaged internal collaborations

Extending the collaboration with the Institute of Biotechnology and Biochemical Engineering could result in the development of other sensors. Providing us enzyme aggregates of different oxidases would allow us to adapt the above presented sensor concept to other relevant analytes.

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CLARA: a Tool for Clustering of Flow Data to Build Compartment Models of (Bio-)Chemical Reactors

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We present CLARA, a tool for the unsupervised clustering of arbitrary multiphase flows into distinct compartments based on open-source tools. Our aim is to enhance the understanding of such multiphase flow systems - prevalent in many chemical and biochemical reactors - by using models consisting of such compartments. The proposed methodology integrates computational fluid dynamics (CFD) simulations with unsupervised machine learning (i.e., clustering algorithms) to identify coherent flow regions (i.e., compartments) without prior labelling. Our workflow is fully automated and designed for reproducibility, with a modular structure that allows an easy adaptation to various flow systems. Our recently published results [1] demonstrate that our approach can successfully capture essential flow features and partition the domain into meaningful compartments. This facilitates direct use in compartment models, which greatly reduces computational costs in larger-scale simulations. Also, compartment models can be combined with modern control strategies to optimize reactor performance during operation, or to realize “soft sensors” [2]. Our findings suggest that unsupervised machine learning algorithms are mature enough to simplify complex multiphase systems in a largely automated fashion, making them a valuable tool for both academic research and industrial applications.

Envisaged internal collaborations

Collaborations with groups that can supply detailed flow data (e.g., from CFD simulations, or local measurements) would be highly welcome to test CLARA. In addition, interaction with researchers that have a use case for modeling (e.g., multiphase reactor that should be modelled, controlled, or optimized with respect to geometry and operating parameters) could help to build new collaborations.

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Dual-Enzyme Crosslinked 3D-Printed Polysaccharide Biomaterials: Enhancing Structure, Mechanics, and Swelling Properties

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The rapid advancement of 3D printing technology has revolutionized the development of polysaccharide-based hydrogels, opening new horizons for tissue engineering and regenerative medicine[1]. In this study, we present the fabrication and comprehensive characterization of 3D-printed polysaccharide biomaterials, employing alginate modified with tyramine and reinforced with nanofibrillated cellulose. Leveraging an innovative dual-enzyme crosslinking strategy-utilizing calcium ions (Ca^{2+}) and horseradish peroxidase (HRP) (see **Figure 1**)-we achieved constructs exhibiting outstanding shape fidelity, mechanical integrity, and dimensional stability[2,3].

The resulting scaffolds were systematically evaluated for their swelling behavior, structural stabilization, mechanical strength, and morphological features. Our findings highlight the remarkable potential of these 3D-printed polysaccharide structures as robust, biocompatible, and highly customizable scaffolds. Notably, their properties closely mimic those of native tissues, such as cartilage and cardiovascular tissue, underscoring their suitability for advanced biomedical applications.

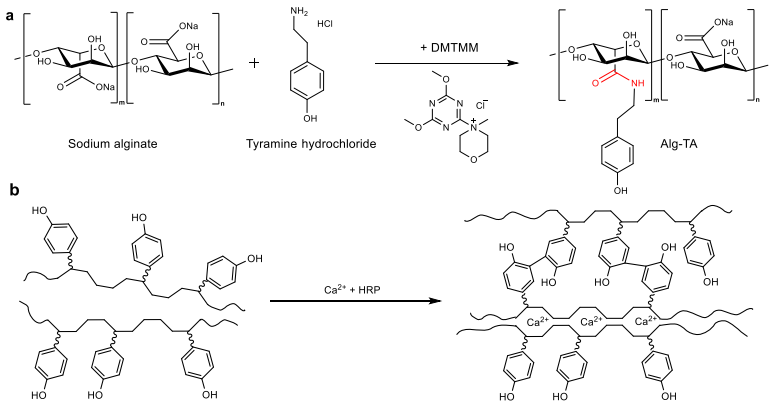

Figure 1. (a) Modification of sodium alginate with tyramine hydrochloride and DMTMM

(b) Ionic and enzymatic crosslinking of modified alginate

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Computational Protein and Enzyme Design

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Computational protein design has been a promising tool for creating superior biological materials with tailor-made properties, new pharmaceuticals, or complex fine chemicals for more than a decade. After demonstrating successful and reliable design of protein structures [1], there has recently been a dramatic increase in protein design methods for the design of functional proteins. This has largely been driven by readily available machine learning (ML) models, which have been adapted to the protein design problem, tremendous reduction in the cost of DNA synthesis, and ever-increasing computational power. De novo enzyme design is the attempt to use our best understanding of protein chemistry and physics – how enzyme active sites pre-organize their catalytically active residues, what their typical intramolecular interactions are, and how the remaining residues stabilize the transition state of a reaction – to identify a minimum energy amino acid sequence composition and geometry that allows the enzyme to efficiently catalyze its reaction. Therefore, reliably introducing function into genetically encodable de novo proteins is still a challenging task. Current design methods mostly produce de novo enzymes with low activities. As a result, they require costly experimental optimization and high-throughput screening to be industrially viable. We are working on, hybrid machine learning and atomistic modelling strategy for scaffolding catalytic arrays in de novo protein backbones and methods to judge the quality of designed protein systems. Recent highlights include the design of proficient enzymes catalyzing the retro-aldol [2,3] and Morita Baylis-Hillman reaction [3], as well as metal cofactors of increasing complexity and methods to enhance recombinant protein production [4].

Envisaged internal collaborations

Potential for collaborations: any exploratory or applied research that involves protein or enzyme engineering, protein stabilization, protein-surface interactions, protein based diagnostics, biocatalysis.

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Scale-Up of 3D-Printed Bioreactors for Continuous-Flow Biotransformation

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The development and optimization of 3D-printed hydrogel-based bioreactors for continuous-flow biotransformations using immobilized cyanobacteria (*Synechocystis* sp. PCC 6803) are presented. The cells, engineered to express the ene-reductase *YqjM*, enable light-driven NADPH regeneration for stereoselective reductions [1]. A nanocellulose/alginate composite bioink was formulated to ensure structural integrity and biological viability under operational conditions [2, 3]. Various reactor geometries were designed and fabricated via extrusion-based bioprinting, with print quality enhanced through custom G-code modifications. Flow dynamics were improved using 3D printed internal structures, and mechanical stability was confirmed through tensile testing. Residence Time Distribution experiments were used to evaluate axial dispersion and flow characteristics, providing key insights that guided reactor design improvements for scale-up [4]. Comparative studies across batch, recycle, and continuous modes demonstrated increased performance under continuous operation. A scaled-up reactor was successfully implemented, confirming the feasibility of integrating photo-biocatalysis with continuous-flow technology. This work highlights the potential of combining 3D printing, biotechnology, biobased chemistry, and process engineering for modular and sustainable biotransformation platforms.

Envisaged internal collaborations

This project is a collaborative effort between the Institute of Process and Particle Engineering (IPPE), the Institute for Chemistry and Technology of Biobased Systems (IBioSys), and the Institute of Molecular Biotechnology (IMBT). Continued collaboration between these institutes could further improve reactor design and scale-up, while addressing current challenges such as long-term stability, mass transfer limitations, and product absorption. By combining complementary expertise in reactor engineering, bio-based materials, and molecular biotechnology, this work aims to advance robust and scalable photobiocatalytic systems.

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Synthesis of organic and hybrid semiconductors and their integration in (opto)electronic devices

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The advancement of next-generation optoelectronic devices strongly relies on the development of new semiconducting materials and their integration into high-performance, stable, and scalable device architectures. In this poster, we present our work in three areas: organic solar cells (OSCs), perovskite solar cells (PSCs), and organic field-effect transistors (OFETs).

For OSCs, we synthesize new non-fullerene acceptors (NFAs) featuring non-fused-ring structures with tailored electron-withdrawing end groups. These NFAs exhibit strong and broad absorption in the visible region of the solar spectrum and well-suited energy level alignment with efficient donor polymers. Devices fabricated with these NFAs show competitive power conversion efficiencies and good long-term stability under illumination.

In the area of perovskite solar cells, we develop novel conjugated organic diammonium iodide A-site cations for quasi-2D perovskites, aiming to enhance charge carrier mobility and power conversion efficiency compared to perovskites prepared with non-conjugated A-cations, while obtaining high device stability. These conjugated diammonium iodides, based on oligothiophene or phenylenevinylene units, lead to well-defined quasi-2D perovskite films. Solar cells based on these materials demonstrate efficiencies up to 13%, and increased out-of-plane charge carrier mobilities were found.

In the field of OFETs, we establish a green synthetic route for the high-mobility small molecule C8-BTBT, avoiding toxic solvents and minimizing waste. Using a scalable solution-based blade coating technique, we fabricated bottom gate top contact OFETs with mobilities up to 1 cm^2/Vs.

These results highlight how targeted material synthesis can enable well-performing and sustainable optoelectronic devices by enhancing specific properties across various technologies.

Envisaged internal collaborations

Collaborations are ongoing with the Institute of Inorganic Chemistry for SAXS and AFM measurements, as well as database management. In addition, joint efforts with the Institute of Analytical Chemistry and Food Chemistry focus on the development of organic semiconductors and dyes.

Synthesis of ApoA1 Mimetics

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Apolipoprotein A1 (ApoA1) is a crucial member of the blood apolipoproteins and serves as a major component of high-density lipoprotein (HDL). ApoA1 has substantial potential as a carrier for small interfering RNA (siRNA) into tumor cells expressing scavenger receptor B1 (SR-B1). Evidence supporting the beneficial effects of ApoA1 in reducing atherosclerosis has been demonstrated through studies where mice were treated with purified ApoA1 and in mice with transgenic or adenoviral-mediated overexpression of the human ApoA1 gene.[1] Considering the anti-inflammatory properties and immune regulatory functions of ApoA1, it is evident that this apolipoprotein has significant potential as an anti-tumorigenic agent.[2] ApoA1 exhibits 90 % amphipathic α-helical content.[2] Helical surface mimetics use conformationally restricted scaffolds with attached functional groups that mimic the i+1, i+2, i+2 and i+5 pattern of side-chain positioning of an α-helix (Figure 1).[3]

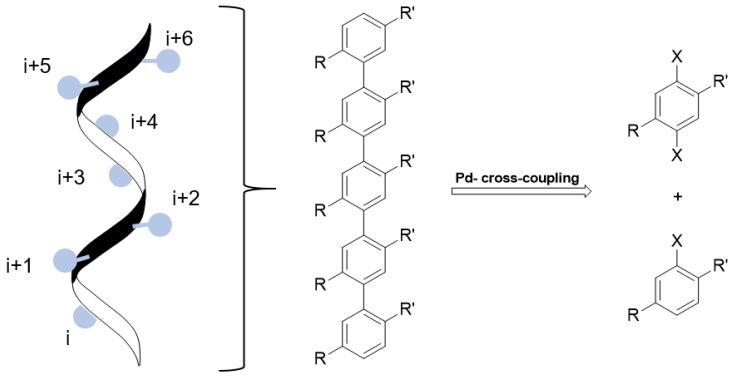

Figure 2: Assembly of pentaryl-based alpha-helix mimetics (R = lipophilic, R‘ = hydrophilic, X = BPin, I).

Previous research on ApoA1 mimetics, which are based on small amphipathic peptides, has demonstrated promising results. However, these mimetics face challenges related to selectivity and stability.[4] Consequently, our group investigated the synthesis of an amphipathic pentaryl ApoA1 mimetic to address these issues. The α-helical structure should be imitated using pentaryls with both hydrophilic and lipophilic side chains (Figure 1). The design is inspired by the structure of ApoA1 and existing peptide-based ApoA1 mimetics.

Envisaged internal collaborations

None

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Iron and Hydrogen: Two Technological Pathways Toward Low-Carbon Energy and Industry

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Chemical Looping Hydrogen for Energy Storage: With growing hydrogen demand as energy carrier and feedstock, efficient and scalable storage is essential. Chemical looping hydrogen (CLH) offers a promising solution for production, purification, and long-term storage [1]. In CLH, hydrogen-containing gases reduce metal oxides, storing energy within the solid phase. Subsequent oxidation with steam restores the material and yields high-purity hydrogen for industrial uses [2, 3]. Material selection is central to performance: iron-based carriers offer high hydrogen yield, low cost, and environmental benefits. Research at CEET focuses on optimizing iron content and inert additives to balance reactivity and structural stability. In addition to material development, CEET also investigates reactor engineering aspects such as design optimization, heat integration, and process control.

Direct Reduction of Mineral Iron Carbonate with Hydrogen: Hydrogen is a key enabler for decarbonizing hard-to-abate sectors such as steel production. One major challenge lies in the reduction of siderite ($FeCO_3$), which conventionally requires a two-step high-temperature process: calcination in air releases CO_2 and forms hematite, subsequently, hematite is reduced in the blast furnace. This approach is energy-intensive and emits significant CO_2 from both stages. CEET developed an alternative process based on direct hydrogen reduction of siderite in a single step at 700–800 °C. This innovation cuts CO_2 emissions by over 60% and reduces hydrogen consumption by 33% compared to the conventional route. In addition, the process gas is upgraded in hydrogen atmosphere by the formation of CH_4 and CO instead of releasing CO_2. By careful selection of the process conditions, a customised process gas can be obtained, in addition to the directly reduced metallic product. [4]

Envisaged internal collaborations

Access to XRD and EDX facilities for advanced material characterization would be valuable for our ongoing research. CEET offers high-pressure TGA measurements and brings expertise in fixed-bed solid–gas systems, which can support collaborative projects.

Acknowledgement

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3D printed scaffolds from turmeric extracts obtained by green supercritical CO_2 extraction

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Turmeric (*Curcuma longa* L.) is a rhizomatous herbaceous plant that is widely used in traditional medicine and functional foods due to its remarkable biological activities. The primary active compounds, curcuminoids, including curcumin, demethoxycurcumin and bisdemethoxycurcumin, have shown antioxidant, anti-inflammatory, antimicrobial and anti-cancer properties [1]. However, their extraction and formulation is challenging due to poor solubility, limited stability and dependence on environmentally harmful organic solvents in conventional processes [2]. In this study, supercritical extractions were performed using supercritical CO_2 (SFE) without the addition of co-solvents. Extractions were performed under different conditions (40–60 °C; 25–35 MPa) to optimize yield and bioactivity. The highest extraction yield was 4.34 wt.% at 60 °C and 25 MPa. The extract obtained at elevated temperature and pressure showed the highest phenolic content and antioxidant activity as measured by the $ABTS^{+\cdot}$ method. The content of curcuminoids was also confirmed in significant amounts (up to 6.6 mg curcuminoids/100 g material) by LC-MS/MS analysis. To improve the application potential and stability of the extract, we have developed a biocompatible formulation using nanofibrillated cellulose (NFC) and alginate [3]. These naturally derived polymers were processed with the turmeric extract into printable inks and formed into scaffolds using a 3D printing process (Direct Ink Writing, DIW). The inks exhibited shear-thinning behaviour suitable for extrusion, and the resulting printed constructs retained their structural integrity. Rheological and mechanical analyses confirmed suitable viscoelastic for biomedical use. In addition, extract in the printed scaffolds showed antimicrobial activity against four clinically relevant microorganisms: *Staphylococcus aureus*, *Escherichia coli*, *Pseudomonas aeruginosa*, and *Candida albicans*, using the microdilution method by minimum inhibitory concentration (MIC). In summary, this integrated and solvent-free approach provides a scalable and environmentally friendly platform for the development of biofunctional curcuma-based materials. Such materials have great potential for applications in wound healing, antimicrobial coatings and personalized healthcare solutions.

Envisaged internal collaborations

Biocompatibility, *in vitro* cell culture, tissue engineering, drug delivery, drug release studies

Acknowledgement

Special thanks are given to the Slovenian Research and Innovation Agency (ARIS) for financial support of research program P2–0046: Separation processes and production design, and scholarship awarded to G.S. Additional acknowledgment goes to the Erasmus+ programme for supporting G.S. in conducting part of the research work abroad through a mobility grant.

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Advances in Synthesis and Biological Evaluation of Ligand Directed Dibromophenyl Ester (LDBP) Probes

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The ligand-directed chemistry (LDC) approach allows site-selective protein labeling of enzymes through proximity-driven covalent modification of an amino acid located near the active site. [1] By using a reversible inhibitor as ligand for protein recognition, the intrinsic activity of the enzyme is restored after the labeling process. Employing various imino- and isoiminosugars as ligand, a comprehensive collection of ligand-directed chemistry probes was synthesized, targeting respective glycoside hydrolases. Based on a synthetic building block concept, different ligands, electrophilic reactive groups, linker moieties and terminal tags can be introduced. [2-4] Biological evaluation of the invented LDC probes gave insights into inhibition profile and labeling properties. Promising candidates were analysed towards their labeling efficiency by intact protein mass spectrometry. The results show, that careful design of each part of the small molecule probe allows selective chemical modification of a specific target glycoside hydrolase. Synthetic details and results from the biological evaluation of synthesised compounds will be given.

Envisaged internal collaborations

For in-depth structural characterization, advanced NMR spectra are measured by Hansjörg Weber from the Institute of Organic Chemistry (TCVB). Intact protein mass spectrometry is performed by Andreas Winkler and Philipp Pelzmann from the Institute of Biochemistry (TCVB) and crystallographic measurements are performed by Roland C. Fischer from the Institute of Inorganic Chemistry (TCVB). Further collaboration is envisioned with the Haas group from the Institute of Inorganic Chemistry (TCVB) and Bernd Nidetzky from the Institute of Biotechnology and Biochemical Engineering (TCVB).

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Synthesis and Materials

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Since the 1960s, research at the Institute of Inorganic Chemistry has traditionally been linked to the molecular and materials chemistry of organometallic compounds of the elements of Groups 14 and 15 of the PSE. The focus has increasingly shifted not only to the synthesis of corresponding derivatives and materials, but also to the characterization of the materials[1].

The topics include synthesis and simulation of precursors for Si- and Ge-based polymers as well as catalysts, energy-relevant materials, clusters, photoinitiators[2], nanomaterials, and their precursors. Furthermore, close research collaborations with industrial partners exist in the field of photoinitiators[2], semiconductor materials, construction materials, and polymeric compounds.

In scheme 1 two examples for cluster as well as P-containing heterocyclic precursor molecules are given.

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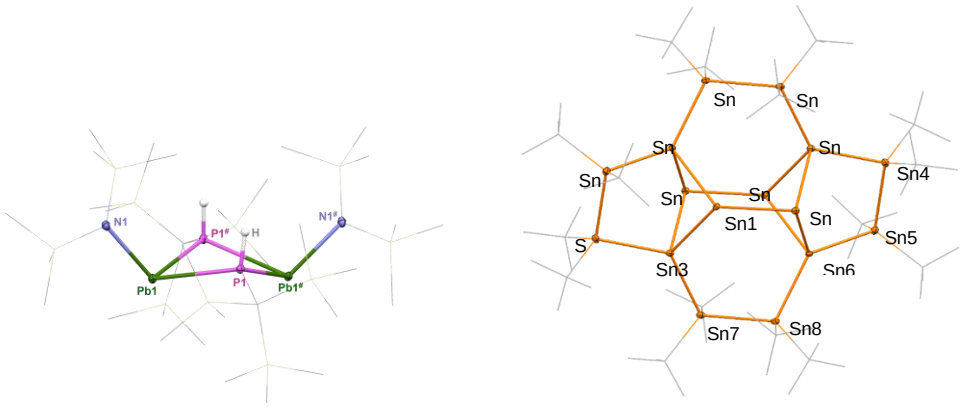

A B

Scheme 1: Crystal structures of a heteroplumbylene (**A**) and a Sn_{16} cluster (**B**) as a model compound for α-tin.

Envisaged internal collaborations

Beside the already existing collaborations within the faculty, we are looking forward to novel research projects with all groups interested in the organometallic chemistry of compounds and materials containing main group elements.

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[2] see poster “Functionalized Hydrosilanes as Next-Generation Precursors for Semiconductor Applications.”; M. Haas

The Soft Matter Application Lab (SOMAPP Lab)

and the SAXS Facilities

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The Soft Matter Application Lab (SOMAPP Lab), a central lab, is a shared project of the Graz University of Technology, Anton-Paar GmbH, and Karl-Franzens University Graz. The project in the area of soft matter analytics was co-financed by the Austrian Federal Ministery of Education, Science and Research within the framework of the "Hochschulraum-Strukturmittel" funds.

The SOMAPP Lab offers research collaborations as well as analytical services for:

Atomic Force Microscope Tosca 400
Density meter DMA 4500 M
Refractometer Abbemat 550
Polarimeter MCP 500
Modular Compact Rheometer MCR 502
Bioindenter UNHT³ Bio
Electrokinetic analyzer for solid surface analysis SurPASS 3
Particle size analyzer Litesizer 500
SAXS-/WAXS-/GISAXS -system SAXSpoint 2.0

The SAXSpoint 2.0 will be upgraded within the next 3 month to provide a better user support.

The TU Graz facility at the Synchrotron ELETTRA (Trieste, Italy) is dedicated to the structural characterization of nano systems with scattering techniques covering topics such as advanced materials, (bio-)polymers, proteins in solids, surfaces, liquids and in the gas phase. The facility provides access to the Austrian SAXS beamline and the Deep X-ray Lithography beamline.

Starting in July 2025 the Synchrotron ELETTRA will be out of service due to a complete refurbishment and upgrade to a state-of-the-art level. During the year 2027 our facility will start operations again providing access to two novel SAXS-/WAXS-/GISAXS beamlines:

High Flux-Beamline (HF-SAXS)
High Brilliance- Beamline (HB-SAXS)

The new High Brilliance-Beamline is a joined project between the University Maribor, the University Primorska, ELETTRA and the TU Graz.

Envisaged internal collaborations

All institutes and working groups of the faculty as well as of the whole TU Graz interested in the above-mentioned techniques.

Soil and Plant Microbiome Engineering for Climate Change Mitigation

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Microbiomes are prevalent throughout the Earth's ecosystems, forming the foundation of food webs and playing a key role in carbon and nutrient cycling. Microorganisms contribute to greenhouse gas emissions and consumption, and in healthy environments, these processes are maintained in balance. However, this equilibrium is significantly disturbed by changing climate conditions and human activities. Our objective is to develop microbial interventions in soils and plants as a strategic approach to mitigate climate change impacts. We are employing technologies such as synthetic microbial consortia, encapsulated plant growth-promoting bacteria (BFC Technology, PCT/EP2018/075760), and plant-microbiome co-breeding methods to address these challenges. Our primary goals include enhancing nutrient use efficiency, increasing soil fertility and carbon sequestration, and improving resistance to existing and emerging plant pathogens. Additionally, we aim to investigate the ecological and functional dynamics of microbiomes under climate stressors such as elevated temperatures, drought, and altered precipitation patterns.

Envisaged internal collaborations

Joint projects could study the combined effects of biologicals and chemicals, such as metal-microbe interactions (e.g., copper), and their influence on nutrient cycling, greenhouse gas emissions, and pollutant degradation. The development of biodegradable delivery systems or matrices for the controlled release of microbial consortia would also be a valuable area of research. Additionally, analysing metagenomes and metatranscriptomes can enhance understanding of mechanisms underlying division of labor in degradation processes, supporting environmental remediation efforts or waste valorization.

Unraveling Ultrafast Li-Ion Dynamics in the Solid Electrolyte $LiTi_2(PS_4)_3$ by NMR Down to Cryogenic Temperatures

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Self-diffusion processes of small atoms or ions play a crucial role in many areas of research. The unique crystal structure of $LiTi_2(PS_4)_3$ (LTPS) presents a variety of energetically inequivalent diffusion pathways for small Li^+ charge carriers and has resulted in one of the highest Li^+ diffusion coefficients. Investigating these pathways individually at the atomic scale poses significant challenges, especially for probing jump processes. In this study, we utilized nuclear spin relaxation techniques down to cryogenic temperatures (10 K) to reveal unprecedented details about both long-range and short-range Li^+ dynamics. The temperature-dependent ^7Li NMR spin-lattice relaxation (SLR) rate exhibits a series of diffusion-induced peaks, allowing the extraction of activation energies and jump rates. Due to the exceptionally fast localized Li^+ exchange processes in LTPS, temperatures as low as 50 K are required to freeze Li^+ dynamics, on the SLR time scale, entirely within the ring-like cages of the LTPS structure.

Envisaged internal collaborations

Calculations of activation barriers or low-temperature properties of crystalline solids needed.

Next generation probiotics for plant and human health: a novel approach to develop microbiome-based biotechnological solutions

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Historically, probiotic applications have primarily involved single organisms. Probiotic development may be enhanced through advancements in metagenome technology and meta-analysis methodologies, enabling systematic identification of microbiome alterations in diseased cohorts. The scientific community has acknowledged the essential role of specific microbial taxa in promoting plant and human health and enabling beneficial functions derived from microbiome research (Berg et al., 2020). Moreover, considering the interconnectedness and exchange of microbiomes across different environments is crucial for global practices such as agricultural management and human medicine. Additionally, this interconnectedness presents potential opportunities to modulate microbiomes to select or promote desirable traits (Sessitsch et al., 2023). We present a comprehensive framework employing a multi-omics approach to identify candidate microbes that may influence plant and human health, based on microbiome data related to what is referred to as next-generation probiotics. The development of next-generation probiotics within this framework has the potential to revolutionize health management. Incorporating emerging insights from microbiome and exposome research, pathogen resistance, host-microbiome interactions, prebiotics, and new bacterial strains into microbiome biotechnology represents a promising frontier within industrial biotechnology.

Envisaged internal collaborations

The Joint project aims to advance the development of next-generation probiotics through strategic collaboration. Joint efforts will focus on genomics, optimizing metabolic pathways, and metabolic modelling to map biosynthetic and regulatory pathways that could enhance the production of beneficial metabolites, such as short-chain fatty acids. Additionally, another collaboration will concentrate on bacterial fungal conservation (BFC) technology, utilizing methods for immobilization and cultivation that improve the long-term survival and metabolic traits of microorganisms, thereby increasing their viability and stability during storage and application. Potential joint efforts may also be directed toward developing biocompatible and functional polymer matrices, as well as conducting process scale-up and stability analyses.

Bibliographic references

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Chemoenzymatic Synthesis of [^{18}F]-Labeled Sakebiose: Towards a New PET Radiotracer for Infection Imaging

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Bacterial infections are difficult to diagnose, especially when differentiating them from sterile inflammation. Certain disaccharides selectively engage bacterial transporters absent in mammalian cells, providing a unique targeting mechanism. However, their diagnostic utility or accuracy is limited by low selectivity in complex biological environments. Radiolabeling disaccharides, particularly with fluorine-18, enhances specificity and enables non-invasive visualization via positron emission tomography (PET), offering a promising strategy for infection imaging.

Among labeled disaccharides, 2-deoxy-2-[^{18}F]-fluoro-sakebiose ([^{18}F]FSK), a fluorinated analog of sakebiose (3-O-α-D-glucopyranosyl-D-glucose), show notable potential as a PET radiotracer for the detection of *Staphylococcus aureus* infections (Figure 1), which are not achieved using the clinical tracer 2-deoxy-[^{18}F]-fluoro-D-sorbitol.[1] Here, [^{18}F]FSK is synthesized from 2-deoxy-[^{18}F]-fluoro-D-glucose via α-1,3-glycosylation catalyzed by nigerose (sakebiose) phosphorylase (EC 2.4.1.279) (Figure 1). To advance utility and clinical translation of [^{18}F]FSK, this project focus on three key directions: **1)** Genome mining and enzyme screening to discover more efficient and stable biocatalysts for enhanced [^{18}F]FSK production; **2)** Transformation of the reaction into a continuous process through enzyme immobilization,[2] enabling separation of biocatalyst from the product and enhancing scalability; **3)** Streamlined clinical-grade purification for future translational studies. Altogether, this project aims to position [^{18}F]FSK as a next-generation, infection-specific PET radiotracer with enhanced scalability, clinical readiness, and diagnostic precision, ultimately contributing to more accurate detection of bacterial infections.

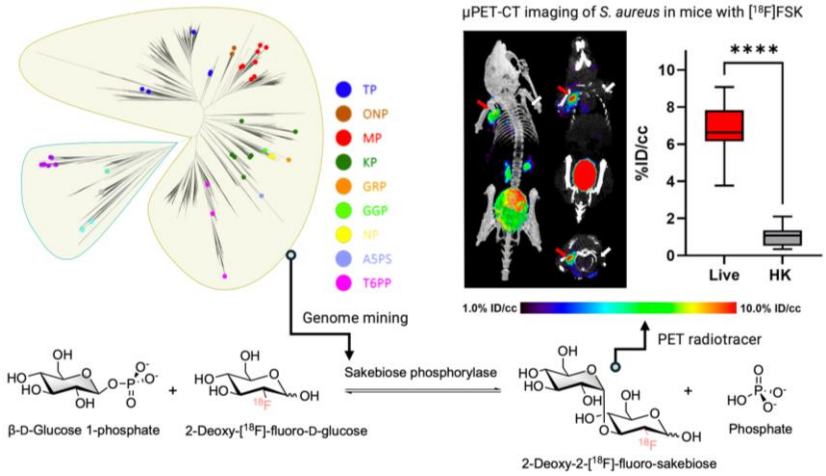

Figure 1. Schematic workflow for the enzymatic synthesis of [^{18}F]FSK as a PET radiotracer for bacterial infection imaging.

Envisaged internal collaborations: collaboration with research groups of biological chemistry and bioprocess engineering could be potentially considered.

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