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Swiss Chemical Society

ALFRED WERNER FUND

MASTER'S STUDENT SCHOLARSHIPS

The Alfred Werner Fund of the SCS Foundation, established in 2013, supports Master degree studies for excellent students from foreign countries in Chemistry or Biochemistry at a Swiss University or at a Federal Institute of Technology. The Foundation offers scholarships in the amount of CHF 30'000 for international students nominated by the partner universities.

Partner Universities / Federal Institutes of Technology

ETH zürich · EPFL · Universität Basel · UNI FR Université de Fribourg Universität Freiburg · Université de Genève · Université de Neuchâtel unine · u b Universität Bern · University of Zurich[UZH]

The program continues the initiatives and projects of the former foundation 'Stiftung für Stipendien auf dem Gebiete der Chemie', also known as the 'Alfred Werner Stiftung'. The scholarship program is supported collaboration by the Swiss chemical and pharmaceutical industry and a number of private donors.

Supporting Companies

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So far, nearly eighty scholarships have been granted to students from over 30 countries, most of them continuing their career in Switzerland. To learn more about the Alfred Werner Scholars, please visit the Gallery of alumni at https://foundation.scg.ch/scholarships/scholar-gallery or download the Alfred Werner Program Impact Report 2013–2021 from the same Web site.

Alfred Werner Master's Scholarships 2022–2024

Given the situation in the Ukraine, Committee of the Werner Fund decided already in March to grant stipends to excellent students from the Ukraine to continue their education here in Switzerland. Through this initiative, eight Ukrainian students from Taras Shevchenko University, Kyiv, and Kharkiv National University started MSc studies at ETH Zurich and EPF Lausanne. Two stipends were covered by private donors.

In addition, the Committee of the Alfred Werner Fund granted stipends to the following international students:

Konstantina Kalliopi Armadorou, EPFL Lausanne
National Kapodistrian University of Athens, Greece
Patrick Domke, EPFL Lausanne
Friedrich-Alexander-University Erlangen-Nuremberg, Germany
Ojaswita Pant, University of Geneva
University of Dehli, India
Nathalie Rowlinson, University of Bern
University of Ottawa, Canada
Alexandru-Tudor Toderaşc, ETH Zürich,
University of Bucharest, Romania
Anna Rosa Masoni, University of Basel
University of Pavia, Italy

Alfred Werner Fund Master's Scholarships 2020–2022

Patricia Brandl
Nationality: *Austria*
Bachelor at: *Technical University of Vienna*
Master at: *EPF Lausanne*
Master thesis supervisor:
Prof. Sereina Riniker (ETH Zürich)

Effect of Stereochemistry on the Conformational Behavior of Mutanobactin D and Synthetic Analogs at Polar/Apolar Interfaces

Mutanobactin D, a lipopeptide macrocycle and secondary metabolite produced by Streptococcus mutans, remains a compound of interest since its discovery, as it can inhibit the biofilm formation of Candida albicans. Recent work is enabling the study of its synthetic analogs' indicating the importance of the stereocenter of the aliphatic tail on the bioactivity and molecular basis of action. Employing molecular dynamics simulations, we investigated the conformational space accessible to mutanobactin D and its analogs to further our understanding of the biochemical mechanism at play.

Mutanobactins are lipopeptide macrocycles produced by *Streptococcus mutans* with demonstrated inhibitory effects on the biofilm formation of the opportunistic fungus *Candida albicans*.[1–3] Experiments have shown that mutanobactin D is the most bioactive of the isolated mutanobactins.[1,2,4] and hampers the mycelial growth of *C. albicans*, which would be necessary for a successful biofilm formation (Fig. 1).[3] However, overall cell viability in the unicellular yeast stadium does not seem to be affected.[4]

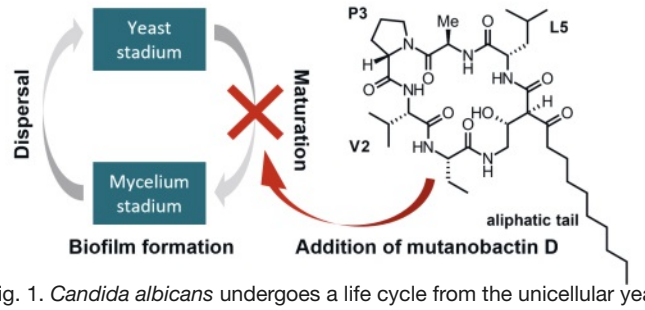

Fig. 1. *Candida albicans* undergoes a life cycle from the unicellular yeast stadium to the maturated mycelium stadium characterized by hyphen growth. This stadium characterizes the pathogenic state and hampers treatment through biofilm formation.[3] Mutanobactin D (on the right with proline, leucine, valine and the aliphatic tail as the prominent amino acids) has been shown to inhibit this maturation process, where the precise biomechanism remains unclear.[1,2,4]

Cyclic peptides – and macrocycles in general – are flexible molecules whose biological functions and physicochemical properties such as cell-membrane permeability largely vary among the different conformations they can adopt.[6] Recent work is enabling the study of the bioactivity and molecular basis of action of mutanobactin D and its synthetic analogs.[5] This demonstrated the importance of the configuration at the site that links the peptidic macrocycle with the lipid chain.[4,5] However, the origin of the structural effects have not been elucidated.

In our work, we set out to characterize the conformational behavior of these lipopeptides in environments of varying polarity to further our understanding of membrane permeability and membrane interactions (Fig. 2).

In addition, we were curious whether we would observe differences in the conformational preferences between bioactive and bioinactive species. To address these questions, we employed molecular dynamics simulations at the polar/apolar interface (serving as a proxy for the cytosol/cell-membrane interface) as well as the monophasic environments.

The insights gained in this manner provide a valuable first step into understanding the biochemical mechanism at play and provide opportunities for experimental validation in the future. More broadly, our work may provide a blueprint for the study and understanding of other lipopeptide antibiotics and their interaction at membranes.

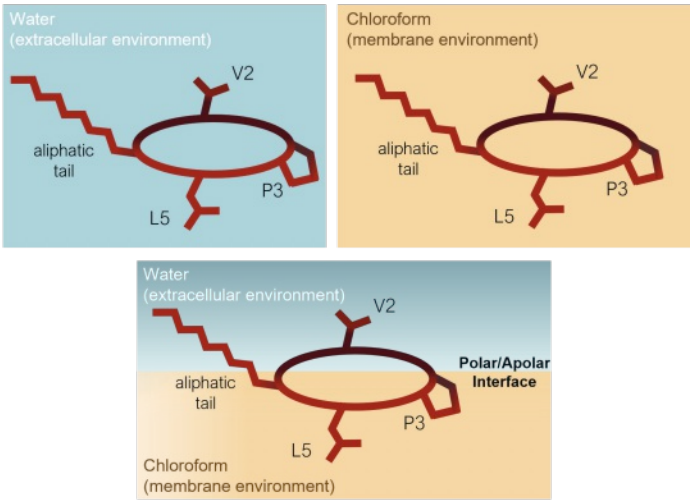

Fig. 2. Experimental setup of the molecular dynamics simulations. We simulated mutanobactin D in monophasic water to mimic the extracellular environment, and chloroform for the membrane environment. In addition, we investigated the accessible conformational space directly at the polar/apolar interface.

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[4] F. Pultar, M.E. Hansen, S. Wolfrum, L. Böselt, R. Fróis-Martins, S. Bloch, A.G. Kravina, D. Pehlivanoglu, C. Schäffer, S. LeibundGut-Landmann, S. Riniker, E.M. Carreira, *J. Am. Chem. Soc.* **2021**, *143*, 10389, https://doi.org/10.1021/jacs.1c04825.
[5] F. Pultar, 'Total Synthesis and Biological Evaluation of Mutanobactin D from the Human Microbiome', PhD Thesis, Zürich: ETH Zürich, **2021**.
[6] A.S. Kamenik, S.M. Linker, S. Riniker, in 'Approaching the Next Inflection in Peptide Therapeutics: Attaining Cell Permeability and Oral Bioavailability',Eds. S.V. Ghodge, K. Biswas, A.A. Golosov, ACS Symposium Series, Vol. 1417; American Chemical Society: Washington, DC, **2022**, pp 137-154, https://doi.org/10.1021/bk-2022-1417.ch005.

Future Steps

After my studies in Lausanne and Zürich, I am now in Basel for an internship at Roche. Since I enjoyed the research that I was able to do during my master thesis a lot, I am considering pursuing a PhD in computational chemistry. However, my dream has always been to not only explore the chemical space, but also the world, so I will take a few months to travel before launching myself into that major next step. Many doors have opened through my studies in Switzerland, which became possible thanks to the support of the Alfred-Werner Scholarship program, and I am excited to see where these will lead me next.

Chiara Compagnoni
Nationality: *Italy*
Bachelor at: *University of Milano-Bicocca*
Master at: *University of Zürich*
Master thesis supervisor:
Prof. Ilija Čorić

Asymmetric Sulfonic Acid Catalysis

Asymmetric strong Brønsted acid catalysis can be considered as one of the most prolific fields in asymmetric catalysis. Since the initial reports by the groups of Terada and Akiyama in 2004, the phosphoric acids and their derivatives have dominated the field of asymmetric Brønsted acid catalysis.[1] On the other hand, the development of chiral sulfonic acids for asymmetric catalysis has been very limited. Our work aims at the synthesis of efficient classes of chiral sulfonic acids.

Despite the long development of the field, chiral phosphoric acids and various derivatives have been leading catalyst structures for strong Brønsted acid catalysis. This can be attributed to their bifunctional activation due to the presence of one Brønsted acidic site (–OH) and one Brønsted basic site (=O), that simultaneously activate the electrophile and the nucleophile, respectively. Sulfuric acid and its organic versions, such as *para*-toluenesulfonic acid, are among the most common strong achiral Brønsted acid catalysts.[2] Sulfonic acids have a higher pKa that could enable the activation of less reactive substrates, such as alcohols and ethers. The potential reasons why chiral sulfonic acids remained largely unexplored is mainly due to two challenges: the presence of two Brønsted basic sites and the more flexible geometry that leads to an open active site and hence limited interaction with the substrates in catalysis. The phosphoric acid moiety can be connected to a chiral backbone through two bonds, placing two bulky groups in proximity to the active site. In comparison, the -SO_3H group is attached through only a single C–S bond and, thus, only one bulky group can be directly covalently bonded to the active site. Additionally, in these structures, the angle between two R groups that provide the chiral environment is at least 120° and therefore wider than in the case of BINOL-derived phosphoric acids. (Fig. 1a)

Furthermore, the attachment through a single C–S bond enables free rotation of the -SO_3H group, which can place the S=O and S-OH moieties in different positions in relation to the chiral environment and thereby further negatively influence the enantioselectivity. Previous attempts at the development of chiral monosulfonic acids have been made by Jakubec, Blanchet, and Enders (Fig. 1b).[3] However, the explored designs are characterized by an open structure around the active site and resulted in lower selectivity compared with the phosphoric acids.

During my work in the group, I optimized the multistep synthesis of a new class of enantiopure sulfonic acids based on a backbone that enables a closed structure. The locked geometry is achieved by installing a larger polyaromatic substituent. The strategy involves using cross-coupling reactions, such as the Suzuki and Kumada reactions, and the insertion of a sulfur atom by a sulfonyl chloride. An important step of the synthesis is the resolution of the catalyst enantiomers through the formation of diastereomers by the attachment of a chiral alcohol (R*OH). The diastereomers can be then separated by classical silica gel column chromatography (Fig. 1c). The final step consists of a Negishi cross-coupling reaction to insert the polyaromatic substituent Ar'', and a simultaneous sulfonate deprotection to directly give the sulfonic acid moiety. (Fig. 1c)

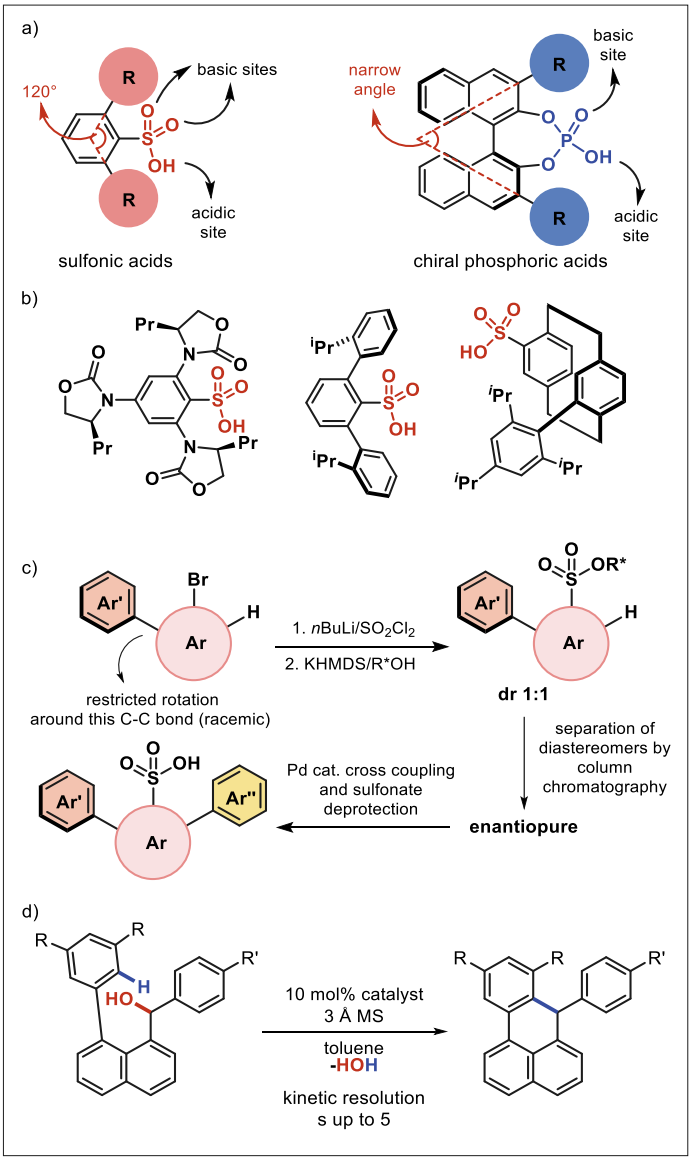

Fig. 1. a) Comparison of the structures of the active sites and chiral environments of sulfonic and phosphoric acids. b) Examples of previous chiral monosulfonic acids.[3] c) General scheme for the synthesis of the sulfonic acids. d) Type of reaction explored to test the catalytic activity.

Several catalysts were prepared by the use of different aromatic components. To test the catalysts and their enantioselectivity, we decided to explore a series of cyclization reactions with aromatic compounds, for example an intramolecular Friedel-Crafts alkylation (Fig. 1d). During this part of my research, I have gained expertise in the parallel setup of asymmetric reactions and analysis by HPLC on chiral columns. I have so far obtained selectivity factors up to 5 for the kinetic resolution process in Fig. 1d.The current work in the group is focused on using the developed synthetic route to access different derivatives for the use in asymmetric reactions, by changing Ar, Ar', and Ar'' groups.

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[2] C. Yang, X.-S. Xue, X. Li, J.-P. Cheng, *J. Org. Chem*. **2014**, *79*, 4340, https://doi.org/10.1021/jo500158e.
[3] a) J. Das, F. Le Cavelier, J. Rouden, J. Blanchet, *Synthesis* **2012**, *44*, 1349, https://doi.org/10.1055/s-0031-1290753; b) D. Enders, M. Ludwig, G. Raabe, *Chirality* **2012**, *24*, 215, https://doi.org/10.1002/chir.21985; c) P. Jakubec, M. E. Muratore, I. Aillaud, A. L. Thompson, D. J. Dixon, *Tetrahedron: Asymmetry* **2015**, *26*, 251, https://doi.org/10.1016/j.tetasy.2015.02.002.

Future plans

I want to thank the Alfred Werner foundation and the Swiss Chemical Society for allowing to pursue my master studies in Switzerland, during which I also did a 6-month internship at Givaudan. After graduating, I am planning on continuing my education by enrolling in a PhD program in organic chemistry with a focus on homogeneous catalysis.

Chung Sum Leung
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Master at: *ETH Zürich*
Master thesis supervisor:
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Electronic Transitions in Orbital Angular Momentum-Carrying Laguerre-Gaussian Beam

Optical vortices (OV) in Laguerre-Gaussian (LG) beam have gained much attention due to its capability of inducing multipole transitions without the need of multi-photon absorption due to its well-defined and separately controllable orbital angular momentum (OAM) and spin angular momentum (SAM), and it has been reported OAM LG beam will enhance the chirality-specific signal sensitivity in chiroptical spectroscopy.[2] To establish a general theoretical framework of OAM LG beam, the nature of multipole transition induced by OAM light was examined through multipole expansion of any electromagnetic wave, accompanying with direct time dependent Schrodinger Equation (TDSE) simulation of the Photoionization of electron from hydrogen with OAM LG beam. The work clarified the multipole nature of an OAM-carrying LG beam in a qualitative way, and served as a pillar of understanding in experimental design which is vital for the future implementation of OAM beam in chiral molecule measurement.

The concept of the angular momentum of the photon has always been one of the major pillars in any field related to electronic transition. The majority of well-studied electronic transitions nowadays can be described based on dipole transition, which corresponds to the transfer of a single unit of angular momentum $\hbar$ between a photon and an electronic system. That single unit of angular momentum is originating from the spin angular momentum (SAM) (correlates to circular polarization) of the photon. However, multipole transition induced by a single photon process is relatively less understood as it requires the photon to carry more than one unit of angular momentum that cannot be described by the spin. The extra units of angular momentum are commonly understood as the orbital angular momentum (OAM) of the light and relating to the topological charge l of the light.

Recent experimental works have demonstrated promising prospects in the application of the OAM light, including control of multipole transition[2] and measurement of chirality-based interaction.[1] Despite the rising attention to OAM light, measurement of the multipole behavior of the OAM light is still non-trivial. Therefore, the objective of the thesis was to develop a theoretical framework through TDSE simulation to understand and predict the light-matter interaction between molecule and OAM LG beam.

Our TDSE simulation successfully predicted the multipole transition induced by OAM LG beam and confirmed the selection rule is simply the summation of OAM and SAM of the incident OAM LG beam:

$|\Delta L| \leq |l| + 1$

With the now established theoretical framework to explain and predict OAM LG beam, we aim to move onto experimental implementation of OAM-based experiment, such Helical Dichroism measurement (Fig. 1) (different chiral response depending the number of OAM of the incident light).

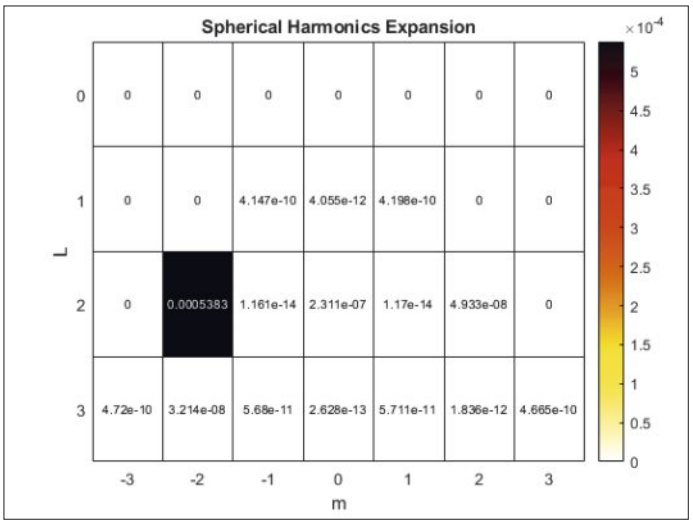
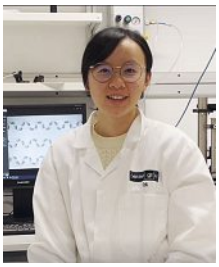


Fig. 1. Spherical Harmonics Expansion of the Electronic Wavefunction after interaction with OAM LG beam (OAM = -1, SAM = -1) in our TDSE simulation. The excited state $Y_{2\text{-}2}$ has the largest transition, which corresponds to quadrupole transition $|\Delta l| = 2$.

[1] W. Brullot, M. K. Vanbel, T. Swusten, T. Verbiest, *Sci. Adv*. **2016**, *2*, e1501349, https://doi.org/10.1126/sciadv.1501349.
[2] C. Schmiegelow, J. Schulz, H. Kaufmann, T. Ruster, U. G. Poschinger, F. Schmidt-Kaler, *Nat. Commun*. **2016**, *7*, 12998, https://doi.org/10.1038/ncomms12998.

Future plans

I recently started my PhD study under the supervision of Prof. H.J. Wörner at ETH Zürich on OAM-related topics using the COLTRIMMS setup.



I-Hsuan Lin
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Bachelor at: *The University of Tokyo, Japan*
Master at: *ETH Zürich*
Master thesis supervisor:
Prof. Andrew deMello

Highly Controllable Microfluidic Gel for Bioprinting

Bioink is a mixture of cells and biomaterials which provide cells with a supportive framework for in vitro tissue or organs growth. It has been increasingly applied in preclinical drug screening because it is more cost effective, reproducible and faster than traditional animal testing. In conventional hydrogel-based bioinks, the exposure to mechanical stress and potential toxicity of cross-linking agents can significantly affect cell function and viability, posing a challenge for researchers. In this study, a new type of bioink with spatially separated cells and linkage matrix was developed. It allows cells to grow in a gentle growth environment, reduces the negative effects of the linkage matrix, and offers the additional flexibility to tune the printability and mechanic properties of the matrix.

3D bioprinting has contributed significantly to tissue engineering and drug testing.[1] It is a process by which cells grow and proliferate in a supportive material and develop cell-laden models, tissue or organs. Here, a bioink consisting of cells and supportive material with special rheological properties can be loaded into a bioprinters, printed out and formed into a designated structure. Desirable bioink features include high printability, great biocompatibility and excellent mechanical properties. In traditional bioinks, hydrogels serve as supportive materials and cells are directly mixed with the matrix and cross-linker.[2] As a result, any modification to the printability and mechanical properties may affect cell viability, proliferation and migration.[3] For instance, increased stiffness has been reported to impede cell migration and reduce cell viability. Therefore, creating a novel structural material that provides desirable rheological properties for bioprinting while maintaining high cell viability is an important task.

In this project, we use microfluidic methods to fabricate a new bioink made up of millions of microdroplets, each of which can encapsulate cells and cell growth media. These droplets form desired gel-like properties through the diverse interaction of their shells. The measurement of G' (storage moduli) and G'' (loss moduli) indicates that our droplet-based gel behaved like a viscoelastic material, in which the gel behaves like a liquid when stressed and like solid when relaxed. The yield points varied with the composition and pH of the outer phase of droplets. The rheological properties of our droplet gels are mainly influenced by the outer phase of droplets, with little effect on the inner phase, giving users the flexibility to tailor the rheological properties of the gel while keeping the cells growing in an optimal state.

Further studies have shown that our droplet gel can be printed in both air and liquid by commercially available 3D bioprinters and is capable of maintaining stable 3D structure for long periods of time (>24 h in air and almost infinite in liquid). Most importantly, based on the proven microfluidic cell encapsulation technology, our droplet gel can provide extremely high cell seeding accuracy and is suitable for a wide range of cell types. Thus, it shows great potential for droplet gels as an alternative to conventional hydrogel-based bioinks.

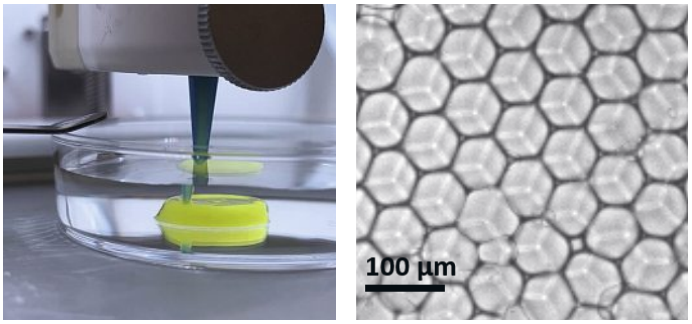

Fig. 1. (a) Image of bioprinting droplet gel in buffer. (b) Microscope image of droplet gel. The droplets adhere and form a beehive structure made up of hexagonal cavities.

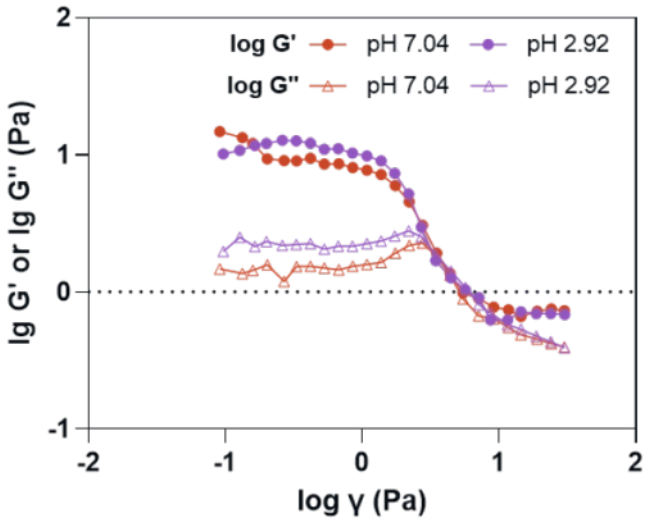

Fig. 2. Rheological measurements of the droplet gels demonstrate the desired viscoelastic properties. The storage moduli and loss moduli are tunable according to gel composition and pH.

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Future plans

I am excited about the potential of microfluidic droplet gels and will have the opportunity to explore their commercialization potential as a research assistant in Prof. deMello's group at ETH Zürich.

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Master at: *ETH Zürich*
Master thesis supervisor:
Prof. Dr. Marco Mazzotti

Assessment of Separation Processes for Capturing Dilute CO_2 from Primary Aluminum Production

There is increasing evidence that swift action must be taken to avoid the most serious consequences of climate change.[1] This entails significantly reducing CO_2 emissions from the industrial sector, which is responsible for a large share of greenhouse gas emissions. However, at the same time as demand for aluminum metal is expected to increase, partly due to growth in solar energy and the electromobility sector, there is currently no mature technology available to produce primary aluminum on a large scale without significant process CO_2 emissions.[2,3] The commercial production process is based on electrolytic reduction of aluminum oxide, using blocks of carbon anodes as a reducing agent, resulting in the release of approximately 1.5 t CO_2/t Al from the smelting alone.[4] Considering the need for sharp emissions reductions to meet international climate ambitions, carbon capture and storage (CCS) technologies may provide a bridging option for decarbonizing the large fleet of primary aluminum smelters worldwide. However, due to a low concentration of approximately 1 vol.% CO_2 in process gases from aluminum smelters, the CCS option has not been studied extensively.[4] Thus, the objective of the thesis was to assess the feasibility of two well-established post-combustion CO_2 capture technologies based on absorption and adsorption to process exhaust gas from primary aluminum smelting.

In the first part of the project, a detailed two-objective techno-economic optimization of an absorption-based capture process using an aqueous piperazine solvent was performed. The objective of the optimization was to simultaneously minimize the process exergy and maximize productivity. This was done by exploiting a connection between ASPEN process simulation software and a Multi-Objective Particle Swarm Optimizer implemented in MATLAB, resulting in the set of Pareto optimal solutions shown in Fig. 1. In the methodology implemented in this work,[5] exergy accounts for the quality of energy required for the separation process (fans, pumps, solvent regeneration, CO_2 conditioning), whereas productivity accounts for the volume of central process units (absorber, heat exchanger, desorber).

The results revealed that the energy requirements for solvent regeneration cause an increase in exergy as productivity increases, whereas other exergy contributions are rather constant. Despite the low CO_2 concentration of the inlet flue gas, reasonable regeneration duties similar to and even lower than those reported for the benchmark monoethanolamine (MEA) solvent were obtained at low to intermediate productivity values and 90% CO_2 capture efficiency. As for the productivity of the process, the volume of the absorber was found to dominate spatial requirements and cause a decrease in productivity with decreasing exergy values. Thus, the results showed that a simultaneous minimization of the absorber dimensions and the duty for solvent regeneration in the desorber are two opposing objectives.

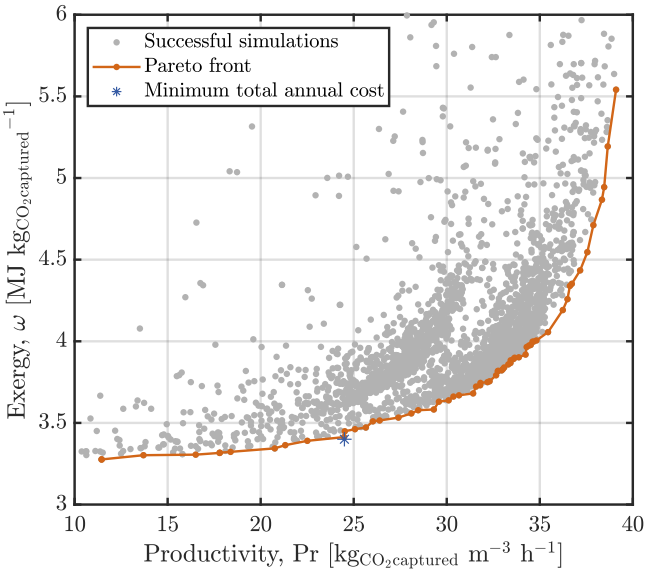

Fig. 1. Pareto front in the ω-Pr plane obtained from the optimization of the piperazine process at 1 vol.% CO_2 in the inlet flue gas and 90% capture efficiency. Results are shown for all successful simulations that converged and met the specifications and constraints of the optimization problem. The point along the Pareto front corresponding to the lowest total annual cost is indicated.

Based on the results of the technical optimization, the total annual cost of the piperazine process was estimated for a reference plant with annual process CO_2 emissions of 0.5 Mt. Among the technically optimal results the minimum cost of capture was found at an intermediate productivity value, ranging from 120–130 EUR/t CO_2 captured.

In the second part of the project, a preliminary technical study of a cyclic CO_2 adsorption process in a packed-bed column using a temperature-vacuum swing for regeneration of an amine-functionalized solid adsorbent was performed. Process simulations were carried out using a Fortran-based adsorption simulation tool, FAST, developed at the Separation Processes Laboratory of ETH Zürich. The results of the analysis revealed that the low CO_2 concentration in the flue gas and the requirement for 90% CO_2 capture efficiency severely restricted the process performance. This led to adsorbent volumes significantly greater than the volumetric requirements of the solvent-based capture process, rendering large-scale application of the adsorption process impractical. More advanced sorbents and cycle configurations could improve the process performance, although handling solids on a large scale is expected to be challenging.

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[2] International Energy Agency, 'Aluminium', **2021**, https://www.iea.org/reports/aluminium.
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[4] S. Broek, S. Save, in 'Essential Readings in Light Metals', Vol. 2, **2013**, pp. 993, https://doi.org/10.1002/9781118647851.ch147.
[5] J. F. Pérez-Calvo, M. Mazzotti, *Int. J. Greenh. Gas Control*. **2022**, 114, 103587, https://doi.org/10.1016/j.ijggc.2022.103587.

Future plans

I would like to convey my sincere gratitude to the SCS Foundation for my selection for this honor. I currently work part-time on CCS as a research assistant in the group of Prof. Dr. Marco Mazzotti, along with my position as Environmental and Sustainability Specialist at Nordural aluminum smelter in Iceland, a subsidiary of US-based Century Aluminum. At Nordural, I will further investigate the potential for CCS in aluminum smelting.

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Master at: *ETH Zurich*
Research project supervisor:
Prof. Dr. Bill Morandi

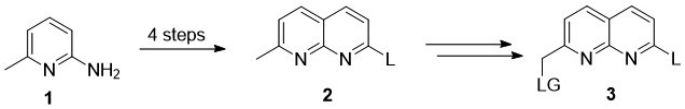
Synthesis of Extended Pincer Ligands for Bimetallic Complexes

A novel unsymmetrical 1,8-naphthyridine-based extended pincer ligand, that could in principle accommodate two different metals or form homobimetallic complexes with two different coordination environments, was synthesized. A monometallic complex was successfully prepared, thus, paving the way for the subsequent addition of a second metal to the remaining coordination site. Such complexes could in general offer unique catalytic activity and broaden the horizons of transition metal catalysis.

Transition metal catalysis has proven to be a very broad and rich field of chemistry. The main reasons accounting for enormous parameter space are the variety of metals available, the ability to fine-tune catalytic activity by appropriate ligand design and the possibility of harnessing metal-to-metal interactions to exert desired chemical activity. The latter remains underexplored in homogenous catalysis due to difficulties in finding the right experimental settings.[1] Since metal–metal cooperativity is very common in heterogenous catalysis and can also be found in various enzymes,[2] development and in-depth research of analogous homogenous model systems would allow for a better understanding of the mechanism of action and the nature of the underlying catalysis behind it.

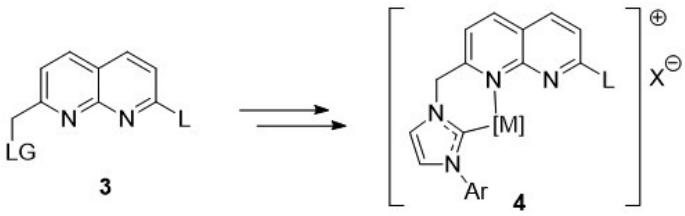
Derivatives of 1,8-naphthyridine are suitable dinucleating ligands due to their rigid, relatively inflexible backbone and various customization possibilities stemming from broad range of potential substituents. Reports about heterobimetallic naphthyridine-based complexes are few and are limited to N- and P-donor ligands.[3] We envisioned a derivative with a coordinating group on one side of the naphthyridine core and a methyl group on the other side that can act as starting point for further functionalization.

The starting material **2** for our unsymmetrical ligands was prepared from commercially available 6-methylpyridin-2-amine **1** in 4 steps (Scheme 1). Functionalization of the methyl group of **2** provided the versatile electrophilic building block **3**.



Scheme 1. Synthesis and functionalization of **2**.

After screening various nucleophiles, the reaction with substituted imidazoles proved to be the functionalization method of choice, thus, introducing an NHC precursor as one of the ligand handles. A variety of *N*-aryl and alkyl substituted imidazoles and different counter-ions were investigated in order to obtain a suitable ligand precursor. Its deprotonation in the presence of a transition metal afforded monometallic complex **4** (Scheme 2), which can be used as a useful starting point for the synthesis of heterobimetallic complexes. The structure of **4** was confirmed by single-crystal X-ray diffraction.



Scheme 2. Synthesis of the metal complex **4** starting from **3**.

With complex **4** in hand, further research will be focused on coordination of another metal to the second binding site with coordinating group designated as 'L' to access the desired heterobimetallic complexes. We envision adding late first-row transition metals, such as Cu, Ni and Co, and consequent screening for catalytic activity.

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Future plans

Soon after the completion of the master's degree I intend to start my PhD studies in the Morandi research group, focusing on various areas of organic chemistry – mechanistic studies, organometallics and development of synthetic methods. I am very grateful to the Alfred Werner Foundation for the scholarship, which enabled me to pursue the exciting and rewarding studies at ETH Zurich, and for providing various opportunities to connect with industry and improve career prospects.