OKV37

Organisk Kjemisk Vintermøte

Thon Hotel Skeikampen, 4.-7. Januar 2024

Otertinden, Foto: Patrick Ihle

NKS

UiT Norges arktiske universitet

FOK

Welcome to the 37th Organic Chemistry Winter Meeting (OKV37)

We are thrilled to have you join us at Thon Hotel Skeikampen for this eagerly anticipated gathering hosted by the Norwegian Chemical Society, Division of Organic Chemistry! This year, our community boasts 111 registered participants from diverse backgrounds in academia, industry, and the institute sector. It is heartening to witness the unwavering support from presenters, attendees, and sponsors, despite earlier concerns raised by industry and academic circles. The committee remains steadfast in upholding the rich traditions of OKV, ensuring another outstanding year.

OKV arguably stands as Norway's most important meeting point for organic chemistry and related sciences, bridging various sectors. The solid track-record of internationally distinguished speakers who have visited the meeting is a quality stamp attesting to our commitment to showcasing cutting-edge research. A second great tradition of OKV is the central role of students (master and PhD) and young postdocs/researchers in the scientific program. Their active involvement underscores our dedication to fostering a supportive environment for learning, networking, and professional growth.

A key highlight of OKV is the active participation of scientific suppliers, vendors, and industry players, offering workshops and invaluable resources. We extend our deepest gratitude to our sponsors for enabling 31 travel stipends, facilitating widespread participation and fostering connections crucial for future careers. Take a good look at the sponsor screen in the lecture hall during the breaks and check out the advertisements and logos in this booklet. We strongly recommend interacting with sponsor stands and exhibitions – they typically have some cool equipment you haven´t seen before, scientific resources and suggestions, competitions with nice prices and always a welcoming smile.

Beyond the scientific program, OKV offers ample opportunities for snow-filled activities, great dining experiences, and engaging social gatherings. The Saturday night banquet promises not just awards for the best presentations and competition winners, but an evening of friendship and celebration. This is the perfect setting to forge lasting connections to the people behind all the scientific scenes and e-mails and learn their perspectives and stories - where you find old and new friends and your future employer, collaborator, customer, and supplier.

Let´s engage and create an exceptional winter meeting together!

On behalf of the OKV37 organizing committee,

Jørn H. Hansen
OKV37 Chairman

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OKV37 Code of Conduct

The 37th Organic Chemistry Winter Meeting in 2024 is committed to fostering an inclusive and welcoming environment for all. We value diversity, equality, and mutual respect in our community and society at large.

Respect for all: We embrace the core principle of respecting and valuing the unique perspectives, backgrounds, and experiences of every individual. Any form of discrimination or harassment will not be tolerated.

Inclusive language and communication: Our communication is grounded in the use of inclusive language and respectful discourse, ensuring that our interactions are considerate and welcoming.

Equal opportunities: We provide equal opportunities for all, without regard to ethnicity, color, gender, gender identity, sexual orientation, religion, nationality, disability, or any other protected characteristic.

Harassment-free environment: We are dedicated to maintaining a harassment-free environment. Harassment in any form, including but not limited to verbal, physical, or visual harassment, is unwelcome.

Looking after each other: We encourage all participants to actively look out for each other's well-being and safety, creating a supportive community where everyone has a responsibility to ensure that others feel seen, safe and valued.

Privacy and confidentiality: We uphold the principles of respecting privacy and confidentiality and do not share personal or sensitive information without explicit consent.

Conflict resolution: In the event of conflicts or disagreements, we encourage open and respectful communication. Seek assistance from the leadership of OKV37, NKS-FOK or NKS if needed (see contact list below).

Accountability: Violations of this code of conduct may result in consequences, including warnings and/or termination of participation in current and future events.

Continuous improvement: We are dedicated to ongoing learning and improvement regarding diversity, equality, and inclusion principles. Let us work together to create a more welcoming and diverse meeting, where each member actively contributes to the safety and well-being of others.

Reporting mechanisms: OKV37 is equipped with a reporting mechanism. If you experience or witness any behavior that violates this code of conduct, please report it to one of the contact persons below (two representatives of the OKV37 committee and two independent contacts). We take all reports seriously and will take appropriate action!

Karina Mathisen (*NKS*)	+47 98673993	Marius Haugland (*OKV37*)	+47 95100355
Anders Vik (*FOK*)	+47 95243996	Annette Bayer (*OKV37*).	+47 95884203


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Program at a glance

Thursday, January 4th	
12:00-15:00	**Arrival, Registration and Lunch. Put up posters**
15:00-15:10	**Opening of OKV37**
15:10-16:10	Invited Lecture
16:10-16:40	Exhibition/Coffee
16:40-17:40	Short Lectures
17:40-18:10	Exhibition/Coffee
18:10-19:30	Short Lectures
20:00	Dinner
Friday, January 5th	
07:30-10:00	Breakfast
08:30-12:00	Snow time
12:30-14:00	Lunch
14:00-15:00	Invited Lecture
15:00-15:20	Exhibitions/Coffee
15:20-16:20	Short Lectures
16:20-17:10	Posters (odd numbers presenting)/Exhibitions/Coffee
17:10-18:10	Invited Lecture
18:10-18:50	Posters (odd numbers presenting)/Exhibitions/Coffee
18:50-19:50	Short Lectures
20:00	Dinner
Saturday, January 6th	
08:00-10:30	Breakfast
10:30-12:00	Snow time/Workshops
12:30-14:00	Lunch
14:00-15:00	Invited Lecture
15:00-15:50	Posters (even numbers presenting)/Exhibitions/Coffee
15:50-16:50	Short Lectures
16:50-17:30	Posters (even numbers presenting)/Exhibitions/Coffee
17:30-18:10	Short Lectures
18:10-18:20	Closing of the Scientific Session
18:20-18:50	General Assembly NKS-FOK (for NKS-FOK members only)
19:45	Aperitif Before the Conference Banquet
20:15	Banquet
Sunday, January 7th	
07:30-10:00	Breakfast
09:00	Bus Departure for the train from Lillehammer to Trondheim
10:00	Bus Departure for the train from Lillehammer to Oslo

The buses cannot wait, so please check-out from the hotel well ahead of bus departure.

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Scientific program OKV37

Thursday	
12:00-14:30	Arrival and Lunch
15:00-15:10	Opening
	Chair: Jørn H. Hansen
15:10-16:10	**Invited Lecture IL-1** **Dr. Kathryn C. Özgün** Project manager at Bayer (Wuppertal) *From Flasks to Fields, Turning Molecules into Medicines & Sustainability in Science*
16:10-16:40	Exhibitions/Coffee
	Chair: Mats Tilset
16:40-17:00	**L-1: Marte Sofie Martinsen Holmsen** (UiO) *Au(III) π-allyl complexes*
17:00-17:20	**L-2: Joseph Lumba** (NTNU) *Because who doesn't love self-healing materials: Reversible Diels-Alder Chemistry in Polymer-Graphene Composites*
17:20-17:40	**L-3: Ashot Gevorgyan** (UiT) *What is the future of homogeneous catalysis?*
17:40-18:10	Exhibitions/Coffee
	Chair: Bård Helge Hoff
18:10-18:30	**L-4: Amalie F. Reinertsen** (UiO) *Stereoselective Synthesis, Configurational Assignment and Biological Evaluations of the Lipid Mediator RvD2$_{n\text{-}3\ DPA}$*
18:30-18:50	**L-5: Karina Ervik** (UiO) *Total Synthesis and Anti-inflammatory Actions of Resolvin D5$_{n\text{-}3\ DPA}$*
18:50-19:10	**L-6: Sigrid Jæger Wexsahl** (NTNU) *Planarization of π-spacers through σ-hole interactions in triarylamine dyes for dye-sensitised solar cells*
19:10-19:30	**L-7: Liza Nguyen** (UiS) *Photodegradable antimicrobial agents*
20:00	Dinner

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Friday	
	Snow time
12:00-14:00	Lunch
	Chair: Marius M. Haugland
14:00-15:00	**Invited Lecture IL-2** **Assoc. Prof. David Margulies** Weizmann Institute of Science *Artificial Communication and Combinatorial Sensing with Molecules that Bind Distinct Protein Partners*
15:00-15:20	Exhibitions/Coffee
	Chair: Magne Sydnes
15:20-15:40	**L-8: Sahra Ahmed** (UiO) *Chiral (N,C,C) Au(III) Pincer Complexes: Synthesis, Characterization and Computational DFT Studies*
15:40-16:00	**L-9: Torfinn Håland** (GE Healthcare) *Chromatography as a purification technique in industrial production on multi ton scale*
16:00-16:20	**L-10: Marcus de Bourg** (UiO) *Synthesis and biological evaluations of epoxy fatty acid mimics*
16:20-17:10	Posters (odd numbers presenting)/Exhibitions/Coffee
	Chair: Trond-Vidar Hansen
17:10-18:10	**Invited Lecture IL-3** **Prof. Joanna Wencel-Delord** University of Würzburg *TBD*
18:10-18:50	Posters (odd numbers presenting)/Exhibitions/Coffee
	Chair: Eirik Sundby
18:50-19:10	**L-11: Marianne Bore Haarr** (University of Dublin) *Enzyme-Triggered Reactions with Transaminases*
19:10-19:30	**L-12: Christian M. Johansen** (Caltech) *Photodriven transfer hydrogenation of N_2 to NH_3 using a Hantzsch esters donor*
19:30-19:50	**L-13: Maria N. Psarrou** (NTNU) *Graphene nanohybrids as sorbent materials for solid-phase extraction of emerging organic pollutants*
20:00	Dinner

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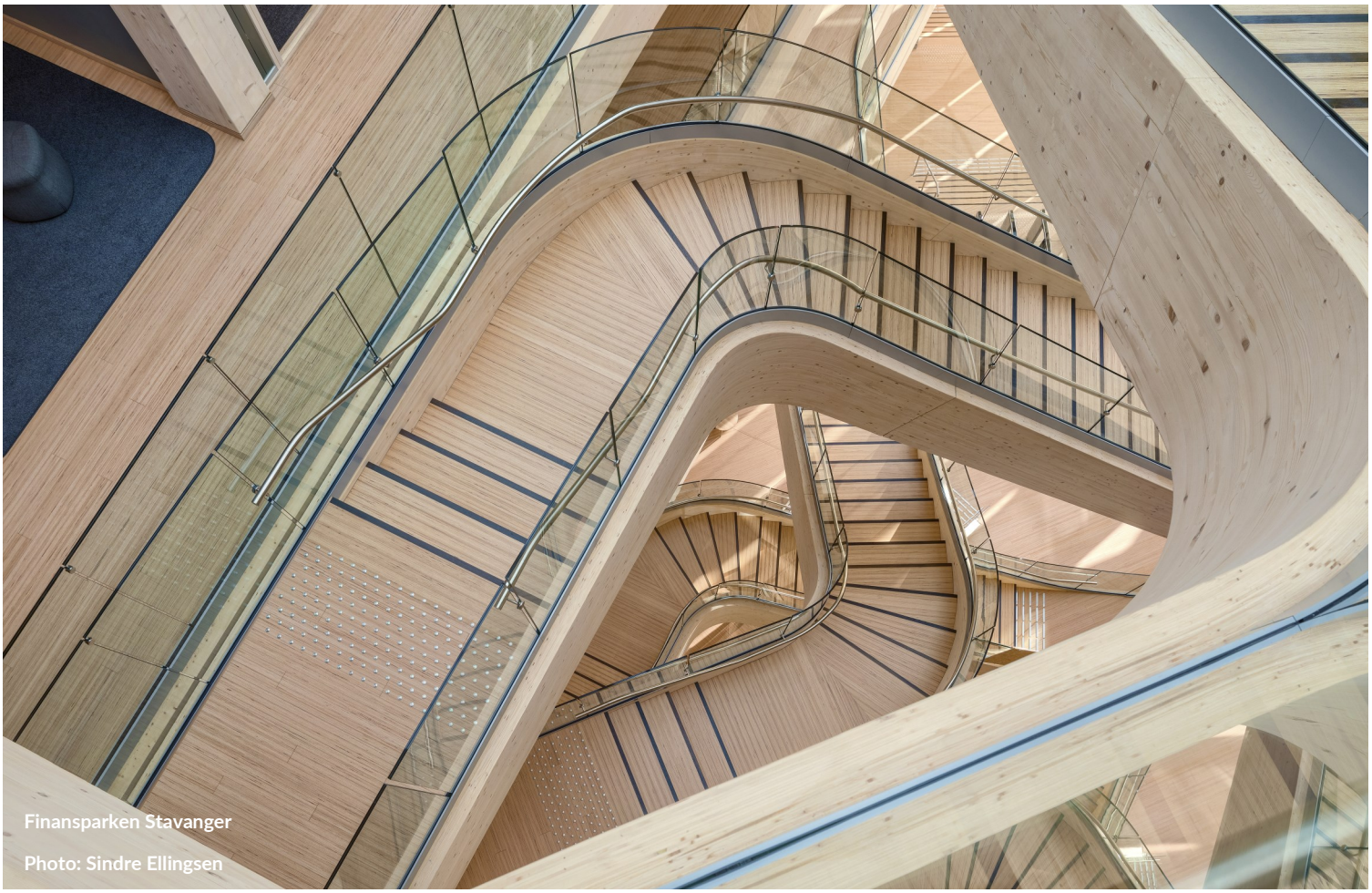
Saturday	
	Snow time/Workshops: ***Elsevier (10:30), CAS (11:15)***
12:00-14:00	Lunch
	Chair: Annette Bayer
14:00-15:00	**Invited Lecture IL-4** **Prof. Jan Deska** University of Helsinki *Exploiting Non-natural Biocatalysis Methodologies as Tools in Organic Synthesis*
15:00-15:50	Posters (even numbers presenting)/Exhibitions/Coffee
	Chair: Bengt-Erik Haug
15:50-16:10	**L-14: Melchizedek Amoakwah** (UiO) *Synthesis and structural characterization of heteroleptic dipyridophenazine–based [Cu(N^N)(P^P)]$^{+}$ complexes*
16:10-16:30	**L-15: Olav Marstokk** (Jotun A/S) *Plant based binders for paint – comparison with fossil-based alternatives*
16:30-16:50	**L-16: Ludvik O. Espeland** (UiB) *Hit discovery for P. aeruginosa pantothenate kinase*
16:50-17:30	Posters (even numbers presenting)/Exhibitions/Coffee
	Chair: Ashot Gevorgyan
17:30-17:50	**L-17: Cecilie Elisabeth Olsen** (NTNU) *Synthesis and evaluation of tetrahydrocarbazoles targeting the β sliding clamp*
17:50-18:10	**L-18: Yomkippur Perez** (UiS) *Unleashing the Potential of Therapeutics: The Promise of Monodisperse PEGs*
18:10-18:20	**Closing of the scientific session by Jørn Hansen**
18:20-18:50	**General assembly NKS-FOK** For members of the Organic Division of the Norwegian Chemical Society only
19:45	Apéritif
20:00	Banquet



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Previous Winter Meetings

Year	Location	Responsible organizer	Institution
2023	Skeikampen	Førsteamanuensis Anders Vik	UiO
2020	Skeikampen	Professor Yngve Stenstrøm	NMBU
2019	Skeikampen	Professor Leiv Sydnes	UiB
2018	Skeikampen	Professor Bård Helge Hoff	NTNU
2017	Skeikampen	Førsteamanuensis Mohamed Amedjkouh	UiO
2016	Skeikampen	Førsteamanuensis Annette Bayer	UiT
2015	Skeikampen	Førsteamanuensis Kåre B. Jørgensen	UiS
2014	Skeikampen	Førsteamanuensis Pål Rongved	UiO
2013	Skeikampen	Førsteamanuensis Bengt Erik Haug	UiB
2012	Skeikampen	Førsteamanuensis Odd Reidar Gautun	NTNU
2011	Skeikampen	Førsteamanuensis Tore Hansen	UiO
2010	Fefor	Professor Rolf Carlson	UiT
2009	Skeikampen	Førsteamanuensis Trond V. Hansen	UiO
2008	Geilo	Professor Leiv K. Sydnes	UiB
2007	Røros	Professor Thorleif Anthonsen	NTNU
2006	Skeikampen	Professor Frode Rise	UiO
2005	Skeikampen	Professor Yngve Stenstrøm	UMB
2004	Røros	Professor Anne Fiksdahl	NTNU
2003	Fefor	Førsteamanuensis Tore Lejon	UiT
2002	Beitostølen	Professor Mats Tilset	UiO
2001	Beitostølen	Førsteamanuensis Hans Renè Bjørsvik	UiB
2000	Geilo	Professor Kjell Undheim	UiO
1999	Geilo	Professor Per Carlsen	NTNU
1998	Fefor	Professor Rolf Carlson	UiT
1997	Fefor	Forskningssjef Odd I. Eriksen	SINTEF Oslo
1996	Fefor	Professor Leiv K. Sydnes	UiB
1995	Fefor	Professor Per Kolsaker	UiO
1994	Fefor	Professor Thorleif Anthonsen	AVH
1993	Beitostølen	Førsteamanuensis Yngve Stenstrøm	NLH
1992	Beitostølen	Professor Leiv K. Sydnes	UiT
1991	Beitostølen	Professor Arne Jørgen Aasen	UiO
1990	Oppdal	Professor Jan Bakke	NTH
1989	Gausdal	Professor Knut Bergersen	UiB
1988	Gausdal	Professor Leiv K. Sydnes	UiT
1987	Fefor	Førsteamanuensis Jan Skramstad	UiO
1986	Bjorli	Professor Thorleif Anthonsen	AVH

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Organizing Committee for the Organic Chemistry Winter Meeting 2024 at Skeikampen

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Associate Professor Marius M. Haugland
Researcher Manuel K. Langer
Postdoc Anna-Luisa Warnke
PhD Candidate Floriane Baussière
PhD Candidate Mateusz Sowiński
PhD Candidate Karoline Nordli
Senioringeniør Truls Ingebrigtsen
MSc student Patrick Ihle

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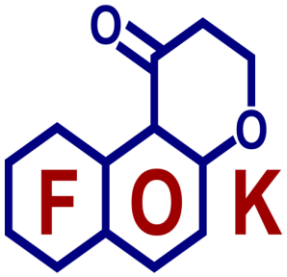

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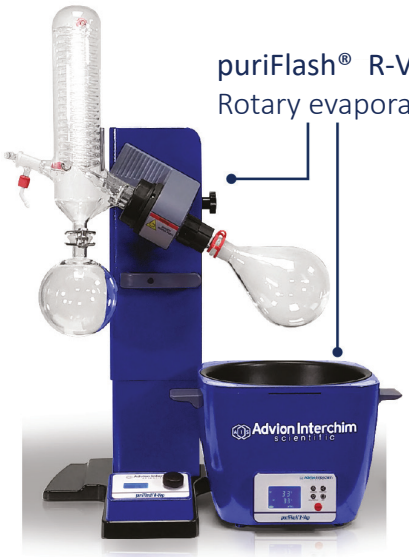

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From Flasks to Fields, Turning Molecules into Medicines & Sustainability in Science

Kathryn Chepiga Özgün[a]

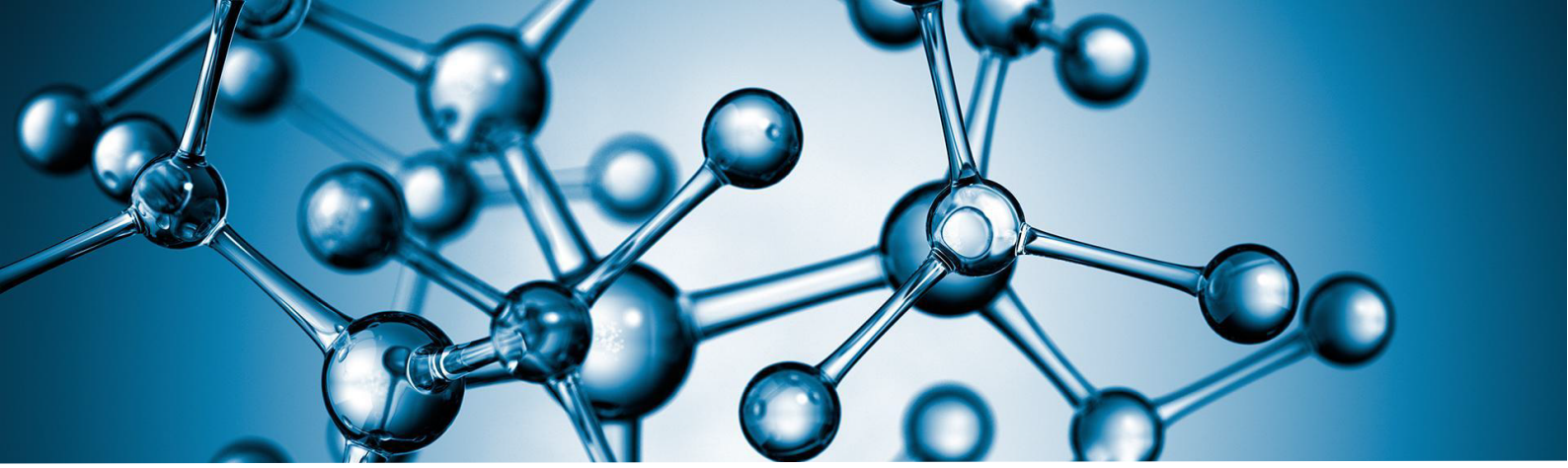
[a]*Pharmaceuticals Division, Bayer AG, Friedrich-Ebert-Straße 217/333, Wuppertal, Nordrhein-Westfalen 42117, Germany*

This talk tells the story of my journey from academia to industry – and the pursuit of sustainable chemistry along the way.

My academic research focused mainly on applying and enhancing dirhodium catalysts. Dirhodium(II) complexes are versatile catalysts for the reactions of diazo compounds, catalyzing a wide array of synthetic transformations. Although dirhodium catalysts can be extremely effective, their cost impedes their use. To address this, we developed a broadly-applicable and highly enantioselective immobilized variant of Rh2(S-DOSP) 4 – the most generally effective chiral dirhodium catalyst for transformations of donor/acceptor diazos. This immobilized Rh2(S-DOSP)4−derivative could be reused over multiple consecutive reactions in batch as well as applied in flow.

Next, the application of dirhodium catalysis in the syntheses of marine alkaloids dictyodendrins A and F will be discussed. These syntheses were achieved by sequential C–H functionalizations utilizing a combination of different C–H coupling methodologies.

Finally, I will share insights into my work at Bayer and describe our sustainability initiatives. One such effort to develop a sustainable process led to the first large-scale application of a Crabtree/Pfaltz-type iridium catalyst for industrial enantioselective hydrogenation. The process optimization for the synthesis of this catalyst will be described.



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Artificial Communication and Combinatorial Sensing with Molecules that Bind Distinct Protein Partners

David Margulies[a]
[a] *Weizmann Institute of Science, Chemical and Structural Biology, Rehovot, 76100 Rehovot, ISRAEL*
David.Margulies@weizmann.ac.il

In this presentation, I will discuss our profound interest in synthetic agents capable of binding distinct proteins and engaging in non-specific, proximity-induced interactions with their surfaces. This interest has led to the development of a novel class of sensors and regulators. The first part of the talk will focus on the design and operating principles of a unique class of fluorescent molecular probes, termed ID-probes,[1-9] which mimic the function of chemical "noses/tongues" (Fig. 1a). Unlike traditional small-molecule-based probes that can detect the presence of a single protein, ID-probes can generate distinct identification (ID) fingerprints for various proteins and their combinations. This unique feature enables these pattern-generating analytical devices to characterize protein subpopulations in biological mixtures and operate within living cells, where conventional macroscopic 'noses/tongues' cannot access. In the second part of the presentation, I will describe the mode of action of synthetic chemical transducers (CTs) that can mediate the activation of enzymes by unnatural protein effectors[10-12] (Fig. 1b). This unnatural protein crosstalk may lead to the rewiring of cell signaling pathways and to the creation of a new class of cell-selective inhibitors whose inhibitory effect in cells is dictated by the cell's environment and consequent protein expression profile. In the final part of the talk, a method by which bacteria can be decorated with artificial, self-assembled synthetic receptors, will be discussed (Fig. 1c).[13-14] This approach, which provides the means to endow bacteria with new properties, enabled the creation of bacterial probes (B-probes) capable of straightforwardly identifying various types of cancer cells.

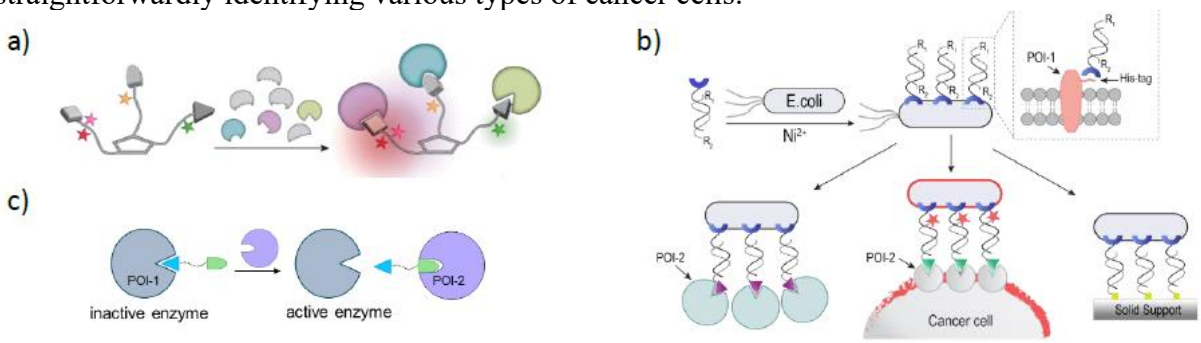

Figure 1. Schematic representation of the main research directions pursued in the Margulies lab.

Selected references:
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Introduction

The Dynabeads team consists of approximately 300 people in Norway. 27% of our employees work in R&D. 47% are millennials. We are currently operating in two locations in Norway in addition to our advanced manufacturing center in Vilnius, Lithuania for bead coupling and finishing.
We hold a full business unit structure with manufacturing, QC, QA, Regulatory, Logistics, Supply Chain, Client Service, Product Management, R&D and Business execution.
Our site has an active leadership team with focus on strategic clarity, Practical process improvement culture, customer intimacy and organization. We are certified as a "Great Place to Work" reflecting our colleagues feeling of trust, pride, and meaningful work in a social and safe environment.
Our Norwegian site has received the Innovation Prize from the Norwegian Research Council in 2017 and the "Norges Smarteste Bedrift" prize in 2018.

What we do

Thermo Fisher's main activity in Norway is the bead business based on the Norwegian invention known as Dynabeads (Ugelstadkuler). The beads are today used in more than 3 billion diagnostic tests worldwide and is an industry standard in sample preparation products in the research market. The beads are world famous for their unique specifications and manufacturing process, which allow use of beads in advanced life science applications. The beads were first used in kits for sample preparations, and today many of the Dynabeads products are still industry standard in cell separation, protein separation, and Nucleic Acid Isolation. Over the last 20 years we have an increasing number of diagnostics customers that purchase beads for use in their diagnostic instrument platforms.

We invest about 80M NOK annually in R&D, and most of our innovations take place in close collaborations with national and international customer projects. The technology is developed and manufactured in Norway. We operate one of the most advanced manufacturing processes in Life Science, and we have a unique competence on both making the beads and the use of beads.

Over the last 7 years the beads have gained great reputation within CAR T-cell cancer immunotherapy after successful results in cancer therapy from collaboration with UPenn University hospital and commercialization of the first Immune Therapy product on the market together with Novartis.
The beads are not only used by external customers, but increasingly more also by other Thermo Fisher business units. The most relevant example is the use of beads on the Ion Torrent Sequencing Chip. The semiconductor chip holds several hundred million microwells, each one containing one highly customized Dynabead where the reaction takes place. Cross functional collaborations like this drives innovation projects of high quality. We also have technology collaborations with Synthetic Biology, One Lambda, Animal Health, and Microbiology.

TBD

Joanna Wencel-Delord[a]

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Exploiting Non-natural Biocatalysis Methodologies as Tools in Organic Synthesis

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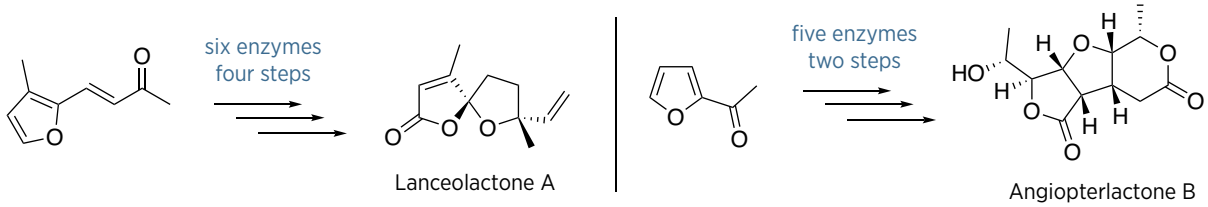
Biocatalysis is increasingly gaining ground as powerful technique in the organic chemist's toolbox for the synthesis of well-defined building blocks. However, with regard to an even broader application of enzyme catalysts in classical synthetic chemistry, the lack of biosynthetic precedence for numerous synthetically relevant reactions and the consequent lack of biocatalysts to promote those reactions need to be considered a major drawback. Since many years, catalytic promiscuity, the enzymes' capability to catalyze fundamentally different chemical interconversions, has been in the scientific focus,[1] however, just recently entirely abiotic transformations came within reach by means of specialized, engineered protein catalysts.[2,3,4]

In our search of biological catalysts with abilities to address synthetically important reactions beyond the biosynthetic repertoire, a range of wild-type metalloenzymes was identified to be effective promoters in a variety of heterocyclic transformations.[5,6] This talk will highlight the synthetic potential resulting from the discovery of enzyme activities in abiotic processes. Focussing on furan oxidation biocatalysis, I will present the enzymatic method development and mechanistic deviations thereof,[7,8] implementations of the novel biocatalysis modules in tailor-made cellular factories for furan valorization chemistry,[9] and applications in natural product synthesis of complex polycyclic plant metabolites such as lanceolactone A[10] and angiopterlactone B.[11]



Lanceolactone A

Angiopterlactone B

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Short Lectures

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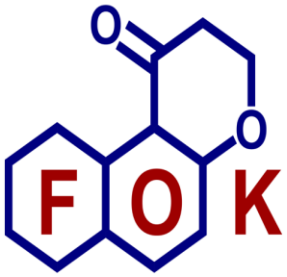

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Au(III) π-allyl complexes

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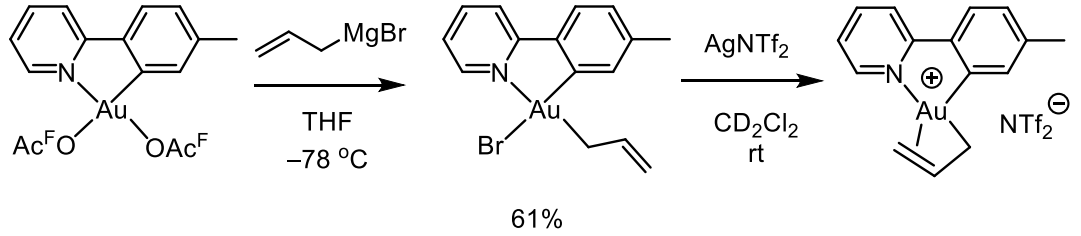
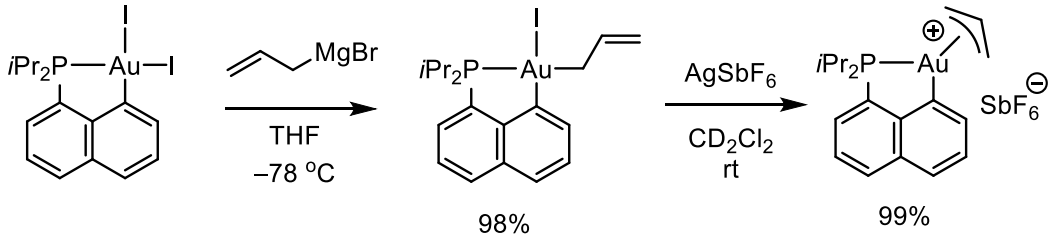
π-Allyl transition metal complexes have been extensively studied. They are key intermediates in many metal catalyzed organic reactions, such as the well-known Pd catalyzed Tsuji-Trost allylic substitution reaction.[1] Despite the large popularity of the π-allyl ligand, Au(III) π-allyl complexes remained unknown until very recently. In 2020, the Bourissou group and the Tilset group independently reported the two first examples of well-characterized Au(III) π-allyl complexes.[2,3] The synthesis, characterization and reactivity of this novel class of Au(III) complexes will be presented.[4]

Tilset:



Bourissou:



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Because who doesn't love self-healing materials: Reversible Diels-Alder Chemistry in Polymer-Graphene Composites

Joseph Lumba[a], Solon Oikonomopoulos[a]

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Stemming from fascination and interest on built-in repair mechanisms in biological organisms, materials science has always been drawn in forming self-healing materials. One noteworthy approach in this domain is the use of reverse Diels-Alder (RDA) chemistry to engineer polymers with intrinsic autonomous healing capabilities. The synthesis involves incorporating dynamic covalent bonds through the RDA reaction, allowing the polymer matrix to undergo reversible cross-linking and de-cross-linking. This field combines various combinations of dienophiles and dienes to modulate reactivity, refining healing kinetics and thermodynamics.[1,2] The intrinsic healing mechanism relies on the dynamic exchange of covalent bonds, responding to external stimuli like heat or light[3], enabling the material to autonomously restore mechanical integrity following damage[4]. In this context, our objective is to explore the application of rDA chemistry in forming graphene-based, self-healing composites. We combine diene-functionalized graphene and dienophile-decorated polyurethane to introduce reversible diels-alder cross-links in the material. We will discuss the challenges and limitations we encountered, as well as further research which can be explored. Finally, we expound on possible practical applications such as reinforcing coatings to enhance durability to the development of aerospace composites with lightweight and self-repairing components.

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What is the future of homogeneous catalysis?

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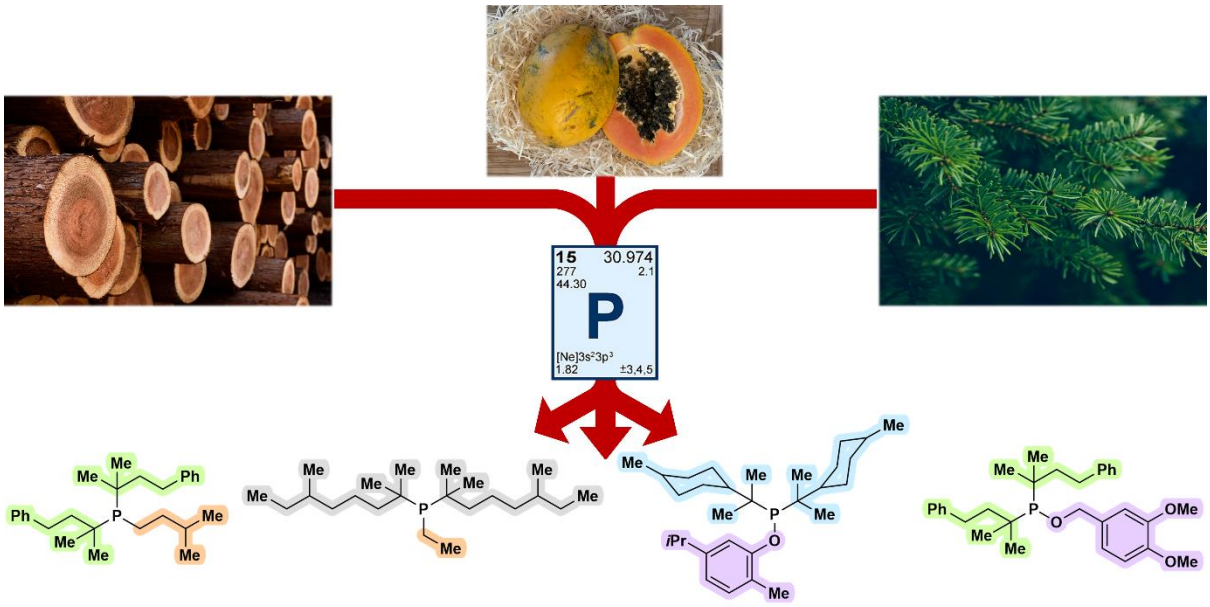
In recent years, biomass conversion into renewable chemicals has made considerable progress. However, the question of whether these resulting renewable chemicals can be transformed into value-added products remains wide open. In this study, we demonstrate that chemicals derived from biomass can serve as viable starting materials for designing phosphine ligands, which can be employed in homogeneous catalysis.[1] Instead of adopting a random approach for ligand design, our strategy involves the targeted development of renewable analogs of a widely recognized and influential phosphine in the field—di(1-adamantyl)-*n*-butylphosphine, alternatively known as Beller's ligand. The developed renewable ligands exhibit high efficacy in several Pd-catalyzed cross-couplings, and the observed results are rationalized by examining their stereoelectronic properties. These developed methodologies can be applied for the late-stage functionalization of commercial drugs.



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Stereoselective Synthesis, Configurational Assignment and Biological Evaluations of the Lipid Mediator RvD2$_{n\text{-}3\ DPA}$

Amalie F. Reinertsen,[a] Karoline G. Primdahl,[a] Roberta De Matteis,[b] Jesmond Dalli,[b] and Trond V. Hansen[a]

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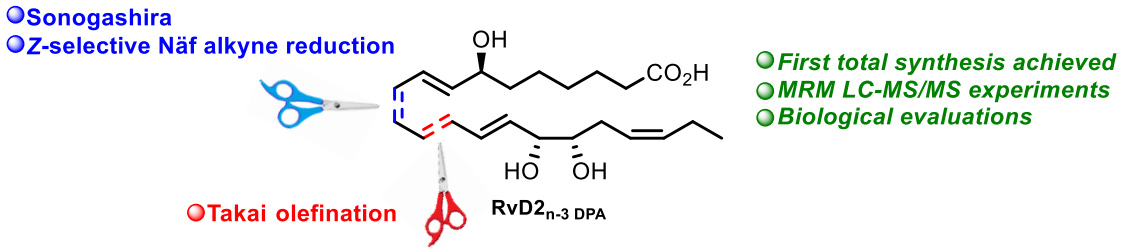
Specialized pro-resolving mediators (SPMs), biosynthesized from n-3 polyunsaturated fatty acids (PUFAs), stimulate the return of inflamed tissue to homeostasis during the resolution phase of acute inflammation.[1] These molecules have demonstrated a range of interesting bioactions as anti-inflammatory and pro-resolving mediators. SPMs are thus highly susceptible lead compounds towards drug development efforts based on resolution of inflammation.

During the last decade, our group has synthesized several SPMs. Recent attention has been on SPMs biosynthesized from n-3 docosapentaenoic acid (n-3 DPA), such as RvD1$_{n\text{-}3\ DPA}$.[2]

The first total synthesis and biological evaluations of the lipid mediator RvD2$_{n\text{-}3\ DPA}$ will be presented.[3]



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Total Synthesis and Anti-inflammatory Actions of Resolvin D5$_{n-3\ DPA}$

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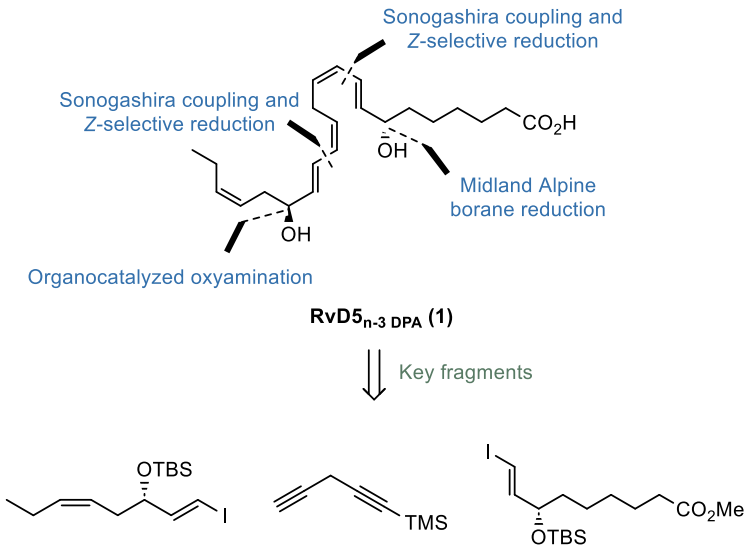
Specialized pro-resolving mediators (SPMs) are oxygenated products of polyunsaturated fatty acids that exhibit pro-resolving and anti-inflammatory biological properties.[1] SPMs are interesting leads for drug discovery based on resolution pharmacology.[2]

In this presentation, the stereoselective total synthesis and biological evaluation of the SPM RvD5$_{n-3\ DPA}$ (**1**) will be presented.[3]



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Planarization of π-spacers through σ-hole interactions in triarylamine dyes for dye-sensitised solar cells

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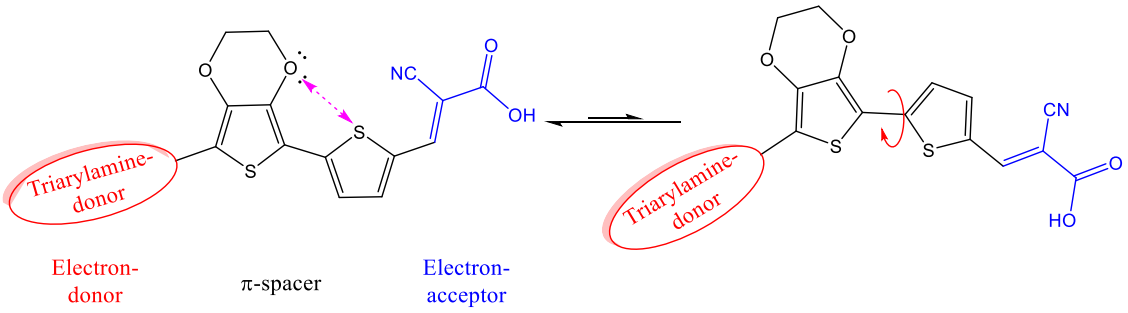
Dye-sensitised solar cells (DSSC) are a form of photovoltaic cell that utilise organic dyes to harvest electromagnetic radiant energy.[1] These organic dyes are usually designed to promote an internal "push-pull" effect that can transport electron density within the molecule.[2] The dyes are often constructed with a donor-π spacer-acceptor design to promote this effect. While all parts of the dye are important to create solar cells with high photovoltaic efficiency, the structure of the π-spacer is critical for an efficient transfer of electron density.

We have synthesised a series of triarylamine dyes to investigate the effect of the geometric structure of the π-spacer. The dyes have a varying degree of planarity in their π-spacers. This planarity was "locked" in using intramolecular interactions between σ-holes, a region of positive electrostatic potential produced by a carbon-sulphur σ-bond, and the negatively charged lone-pair of oxygen.[3,4]



Both the synthesis and the optical properties of the dyes, in addition to the photovoltaic properties measured of the DSSC's created with the dyes, will be presented.

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Photodegradable antimicrobial agents

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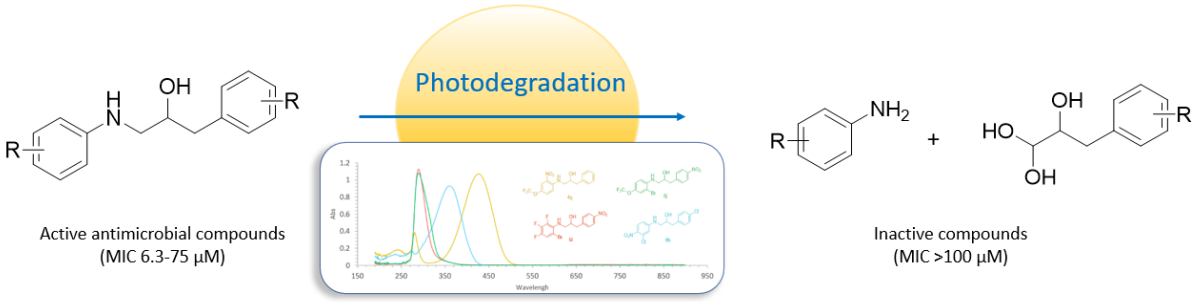
Antibiotic resistance remains a major menace and stands among the most significant threats to public health worldwide.[1] As a direct result of constant exposure of bacteria to active compounds in nature, many strains have become very robust to modern drugs and with no new classes of antibiotics developed recently, it is crucial to develop alternative tools for combating bacteria without triggering resistance.[2]
The idea behind light-sensitive antimicrobial compounds is to reduce the contamination of nature with active molecules after they have been excreted from the patient. Based on a previous study carried out by the group,[3] we demonstrated the synthesis of antimicrobial compounds containing an ethanolamine core that can undergo degradation by light.[4] The biological activity was studied and eight of the ethanolamines described have significant antimicrobial activity (minimum inhibition concentration (MIC) 6.3-75 µM) and are also capable of decomposing under light into fragments that have no antimicrobial activity (MIC > 100 µM).[4]



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Chiral (*N,C,C*) Au(III) Pincer Complexes: Synthesis, Characterization and Computational DFT Studies

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Previous studies on chiral Au(III) pincer complexes as catalysts in asymmetric transformations have shown promising results.[1] In this work, novel bicyclometalated (*N,C,C*)-Au(III) complexes with ligand-based chirality have been synthesized and characterized using an array of techniques including extensive multinuclear NMR spectroscopy, ESI-MS, UV-Vis spectroscopy, and SC-XRD. A new synthetic method was developed to afford prochiral chelating ligands prepared using a combination of the palladium-catalyzed Suzuki-Miyaura cross-coupling reaction and the iron-catalyzed Kumada reaction.[2][3]

The production of a chiral center adjacent to the gold atom results in the formation of a racemic mixture, and resolution was attempted *via* halide abstraction from the (*N,C,C*)-Au(III)-Cl complexes using a chiral silver carboxylate to form a diastereomeric complex. Enantioseparation of the (*N,C,C*)-Au(III)-Cl complexes was also carried out chromatographically using chiral HPLC, and the enantiomeric excess of the racemates was assessed.

NMR studies revealed the formation of several Au(III) species upon the initial coordination attempts, including the desired tridentate (*N,C,C*)-cyclometalated pincer complexes. Using DFT calculations, the thermodynamic stabilities of the various complexes formed were investigated computationally.

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Chromatography as a purification technique in industrial production on multi ton scale

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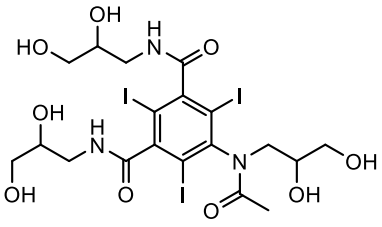
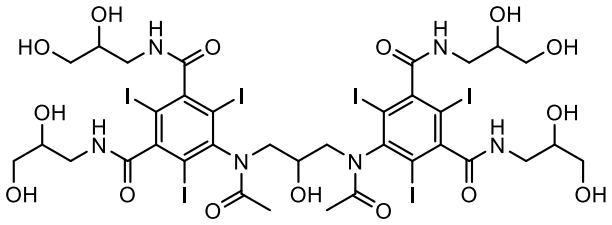
X-ray contrast agents are important in medical diagnostics, and have played a significant role in obtaining enhanced visual insight in to the body for doctors worldwide during the last 40 years. Nyegaard&Co was a pioneer company with research and production in this field. The company became Nycomed and later Amersham, and is now GE HealthCare.

GE HealthCare, Lindesnes Site, produces the active substances used in two of the most known X-ray contrast agents, iohexol (Omnipaque®) and iodixanol (Visipaque®) (structures shown below). The products are produced in large quantities because one patient dose requires typically 50-100 g of contrast agent, and they are used 3 times pr. second worldwide. They contribute to saving lives every day.



Iohexol



Iodixanol

Crystallization is the most widely used purification technique in API production in pharmaceutical industry. This is also the case at Lindesnes Site. In an ongoing R&D project it is, however, investigated whether a crystallization can be replaced by chromatography for purification. This has opened an opportunity for replacing a hazardous organic solvent with water in the synthesis step. In turn this pave the way for a much greener industrial process with much less CO_2 emission and energy consumption.

As X-ray contrast agents are considered as medicinal products, the manufacturing processes have to be registered and approved by regulatory authorities. Changing solvent in the synthesis and going from crystallization to chromatography as a purification technique are fundamental changes that need to be approved by the authorities before industrialization of the new chemical process. Therefore, it is required to show that these changes do not affect the purity profile negatively. This aspect has been studied extensively in this project by using different analytic techniques and methods.

In the lecture the background for the project will be outlined, some highlights from the research will be presented, and some findings from the analytical work will be discussed.

Synthesis and biological evaluations of epoxy fatty acid mimics

Marcus de Bourg[a], Rawand S. Mohammad[a], Abhishek Mishra[b], Ashraf El-Meanawy[d], Jawad Bin Belayet[d], Bruce D. Hammock[c], John D. Imig[b], Mitchell Watsky[e] and Anders Vik[a]

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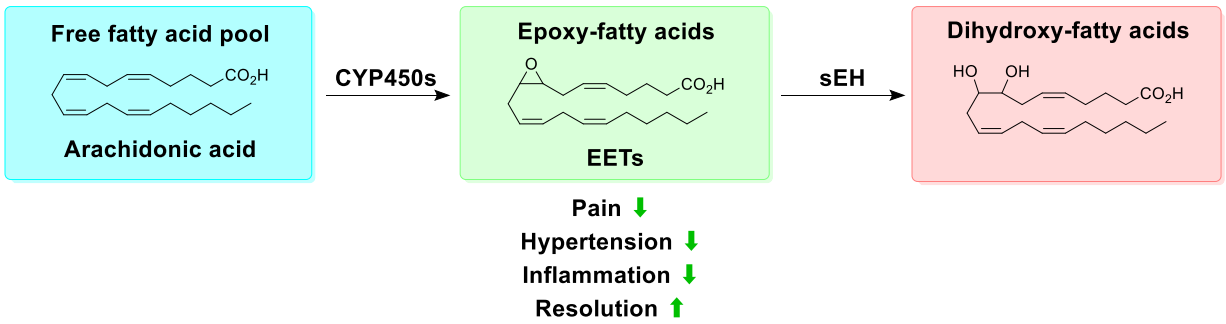
Epoxy fatty acids (EpFAs) are linked to several bioactions in the body. Some of these include pain-relief, anti-inflammatory effect. However, several biological pathways quickly degrade the EpFAs, with the dominating mechanism being epoxide hydrolysis by the enzyme soluble epoxide hydrolase (sEH). Increasing EpFA concentrations through inhibition of the sEH has shown to reduce the severity of a variety of disease states in laboratory settings.[1] In particular, 19,20-epoxydocosapentaenoic acid (19,20-EpDPA) and 8,9-epoxyeicosatrienoic acid (8,9-EET)[2] has proved effective at improving a variety of disease states *in vitro*.

The focus of this project is the synthesis and biological evaluation of potential EpFA mimics that are stable towards sEH. A total of 28 stable potential mimics of 8,9-EET and 19,20-EpDPA have been synthesized. Several of these candidates have been shown to be effective in *in vitro* inflammation models.



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Enzyme-Triggered Reactions with Transaminases

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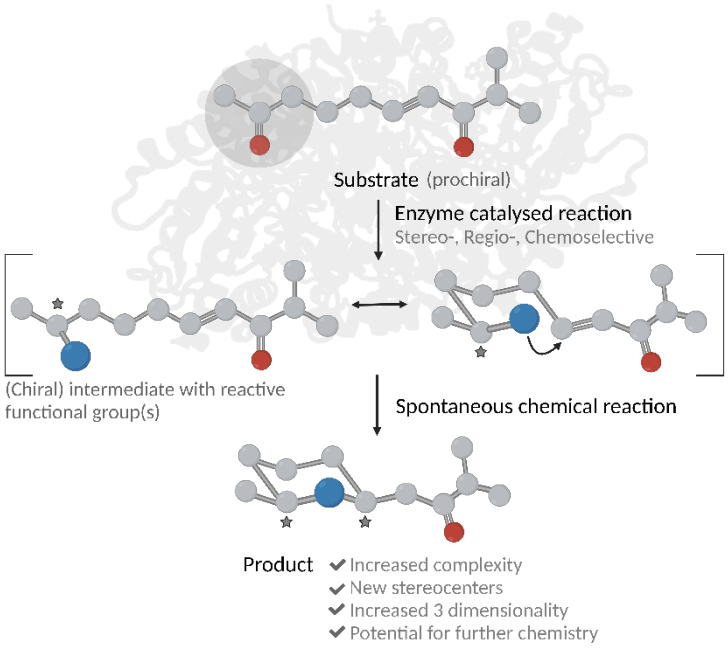
The construction of complex chiral molecules has been a great challenge undertaken by synthetic chemists over the last decades. However, many asymmetric syntheses rely on lengthy reaction pathways including the use of diverse reagents and organic solvents, various protecting group strategies, and/or multiple work ups and purifications. Enzyme-triggered reactions are a powerful approach for building molecular complexity and three-dimensionality from simple, easily accessible starting materials, in a single transformation, with no requirement for protecting group manipulations (Scheme 1).[1]

The capability of a transaminase to catalyse the reversible ketone to amine transformation renders the enzyme an excellent tool for triggering spontaneous reactions that lead to complex chiral molecules.[2,3] The examples highlighted in this presentation showcase the synthetic power of designing smart substrates for enzyme-triggered reactions and their application for the preparation of structurally complex three-dimensional small molecules.



Scheme 1

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Photodriven transfer hydrogenation of N_2 to NH_3 using a Hantzsch esters donor

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Photoredox catalysis is often utilized in small molecule transformations and organic synthesis, however previously there were no examples of molecular photodriven catalytic nitrogen reduction (N_2R; $N_2 \rightarrow NH_3$). Noting that a reduced Hantzsch ester (HEH_2) can behave as 2 e^-/2 H^+ photoreductant, we have shown that, when partnered with a suitable catalyst (Mo), and an organic buffer (collidinium triflate/collidine) under blue light irradiation, HEH_2 facilitates delivery of successive H_2 equivalents for the 6 e^-/6 H^+ catalytic reduction of N_2 to NH_3. Interestingly, while the addition of an iridium photoredox catalysts boosts the yield, unusually an explicit photocatalyst is not required. Mechanistic studies show that in the absence of a photocatalyst the pairing of HEH_2 with the collidine buffer is critical, and upon excitation of HEH_2, collidinium triflate is reduced to generate collidinyl radicals with weak N−H bonds capable of reducing a range of inorganic and organic substrates, in addition to the initially studied N_2R.

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October 14th 2022

Graphene nanohybrids as sorbent materials for solid-phase extraction of emerging organic pollutants

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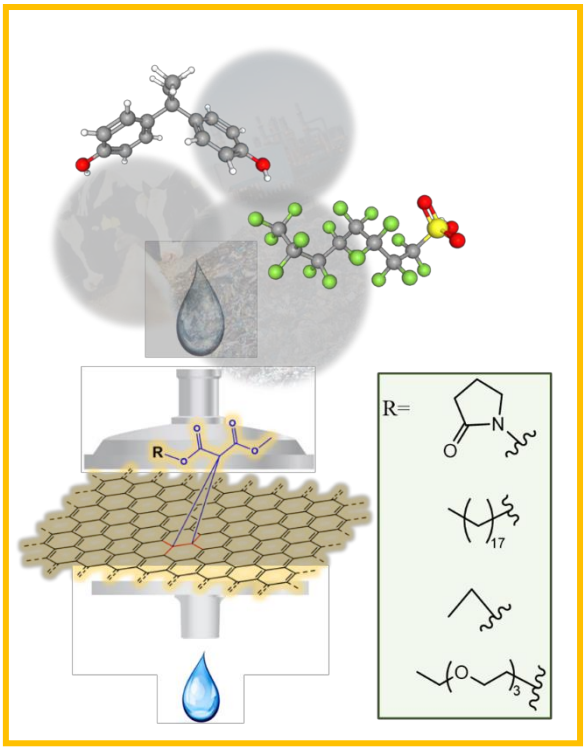
Four different graphene hybrids were evaluated as sorbent media for solid-phase extraction of trace organic impurities present in aqueous samples. The graphene used in the study was exfoliated in N-methyl pyrrolidone by sonication assisted liquid phase exfoliation using a tip probe. The synthetic work involved, first, the syntheses of three novel malonate derivatives bearing octadecyl, N-methyl pyrrolidone and triethylene glycol monoethyl ether and then the Bingel-Hirsch reaction of each derivative with the graphene sheets in the presence of carbon tetrabromide and 1,8-diazabicycloundec-7-ene at 120°C. The fourth graphene hybrid was synthesized with commercially acquired diethyl malonate in the same manner. The nanohybrids alongside unfunctionalized graphene were exposed to water samples containing target analytes of emerging organic pollutants comprised of benzophenones, bisphenols and perfluorinated compounds. The recoveries were measured with LC-MS analysis and the results were very promising to utilize the synthesized nanohybrids as sorbent materials.



Synthesis and structural characterization of heteroleptic dipyridophenazine–based $[Cu(N^N)(P^P)]^+$ complexes

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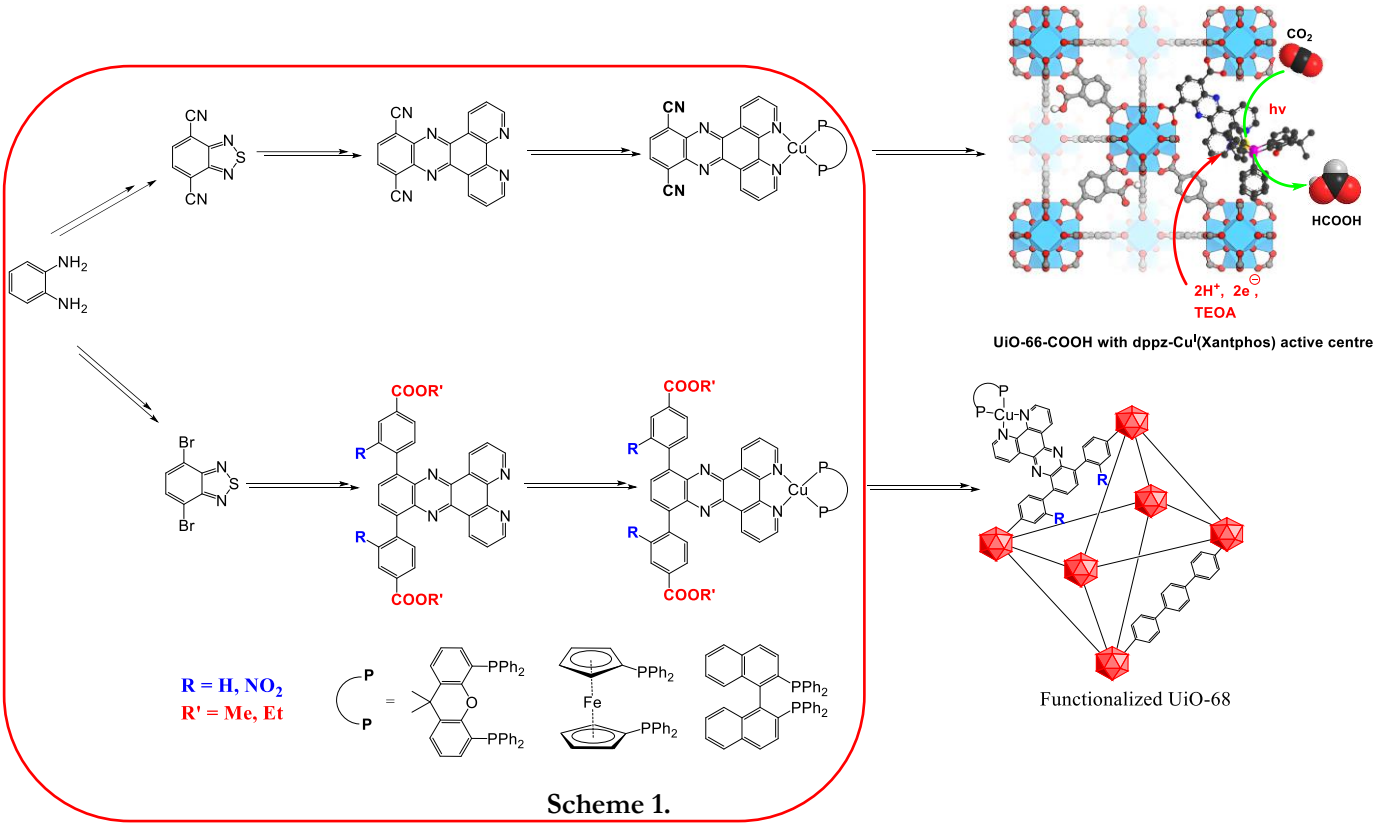
For the purposes of solar–induced multi–electron storage and charge transfer reactions, heteroleptic $[Cu(N^N)(P^P)]^+$–type copper(I) complexes where (N^N)= diimine ligand and (P^P)= bulky diphosphine ligand, have become promising and viable alternatives to noble metal photosensitizers.[1]

The synthesis, structural and geometrical configurations of a series of electron–withdrawing *para*–substituted dipyrido–[3, 2–a: 2', 3'–c]phenazine(dppz) copper complexes (inclusive of the non-substituted) are herein presented (red in **Scheme 1**). With bromo, cyano and 4–methoxycarbonyl nitrophenyl as the substituents and (9,9-Dimethyl-9*H*-xanthene-4,5-diyl)bis(diphenylphosphane) (xantphos), 1,1'-Bis (diphenylphosphino)ferrocene (dppf) and ([1,1′-Binaphthalene]-2,2′-diyl)bis(diphenylphosphane) (binap) as the (P^P) ligands, the corresponding complexes were synthesized via a one–pot two–step method and characterized using multinuclear NMR, DOSY, FTIR and UV–Vis DR spectroscopy.[2]

The dppz ligands were obtained in quantitative yields via bromination, cyanation and Suzuki–type coupling reactions conducted on an intermediate benzothiadiazole scaffold. The cyano and alkyl benzoate derivatives were chosen for the prospective aim of incorporating the complexes into Zr–based MOFs UiO–66 and UiO–68 respectively. The free bromo– and cyano–dppz ligands exhibited severe solubility issues, with NMR characterization being possible upon strong acid addition. The complexes showed satisfying stability upon exposure to air and water with DOSY studies in *N*–donor solvents showing the fortunate absence of dissociative speciation and ligand exchange reactions leading to the formation of homoleptic species. Through–space correlations and solid–state structures defined by NOESY/ROESY NMR and SC–XRD indicated π–stacking properties among the complexes caused by a distorted tetrahedral coordination sphere around the Cu^I metal. From the UV-Vis DRS studies, it was inferred that the presence of *para*-substituted EWGs on the distal benzenoid ring promoted red-shifting of the absorption properties for both the ligands and complexes within the visible region.



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Plant based binders for paint – comparison with fossil-based alternatives

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Email: olav.marstokk@jotun.com

Jotun is a large producer of paint and coatings. Paint and coatings are mixtures of binders, pigments, fillers and additives. The binder, or organic polymer defines the key properties of the coating including durability. An important class of binders are alkyds which are fatty acid modified polyesters. Jotun is developing and producing these polymers in Sandefjord. Currently these polymers are made with raw materials from the petrochemical industry, they are fossil-based.

As part of providing solutions for a more sustainable future, Jotun has launched the Green Steps initiative with concrete goals for reducing our impact on the environment. As part of this initiative, we have projects looking into using monomers having lower carbon footprint. Thus, helping us achieve our goal about reducing greenhouse gas emissions.

Trees are a good source for plant-based (renewable) raw material for the chemical industry. When switching to a renewable source for raw materials sometimes the same chemicals can be made, in other instances we must work with new chemistry. We have investigated both routes. In this paper we will present how we can get monomers for our polyester from plant based raw materials. Several polymers made with plant-based raw material were synthesised and subsequently tested in paints. How do the plant-based ones perform compared to the fossil-based ones? Results from characterization and testing of polymers and paint will be presented correlating the structure of the different monomers with the properties of paint.

Hit discovery for *P. aeruginosa* pantothenate kinase

Ludvik O. Espeland[a,b], Charis Georgiou[b], Ying Ho Leon Lee[b], Samuel Sutton[b], Jørgen Høiem Flornes[a], Bengt Erik Haug[a], Ruth Brenk[b]

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The discovery of antibiotic drugs is evidently among the greatest triumphs of modern medicine, vastly improving the chances of recovery from most common bacterial infections. Today, the fanfares of triumph have modulated into a cacophony of alarm bells, as the efficacy of these drugs are diminishing, and the once dwindling mortality rising. One estimate puts the global 2019 deaths attributed to antimicrobial resistance at 1.27 million, more than malaria and HIV combined, making it among the currently gravest threats to public health.[1] A pathogen of particular concern is carbapenem-resistant *P. aeruginosa*, a highly adaptive Gram-negative bacteria, for which the WHO has declared an urgent need for new antibiotics.[2]

Pantothenate kinase (PanK) is responsible for the phosphorylation of pantothenate, the initial and in some bacteria rate limiting step in the biosynthesis of coenzyme A (CoA). The overall pathway is conserved throughout life, as CoA and its thioester derivatives are central components of ubiquitous metabolic pathways such as fatty acid synthesis, tricarboxylic acid cycle and polyketide synthesis. *P. aeruginosa* utilizes the PanK type III variant, which several studies have found to be essential.[3,4] Inhibitors targeting the type I and II isoforms have been identified, but do not bind to the type III variant due to its narrow binding site.[5] Encouragingly, however, a binding pocket analysis deemed the target druggable.[6]

On this basis we directed our structure-based hit discovery efforts towards *P. aeruginosa* pantothenate kinase type III, using a combination of virtual screening, bio-layer interferometry for hit validation and subsequent X-ray crystallography for binding mode elucidation, a platform we earlier implemented for *P. aeruginosa* β-ketoacyl-ACP synthase II.[7] This endeavor has resulted in a number of hits with potential for further optimization.

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Synthesis and evaluation of tetrahydrocarbazoles targeting the β sliding clamp

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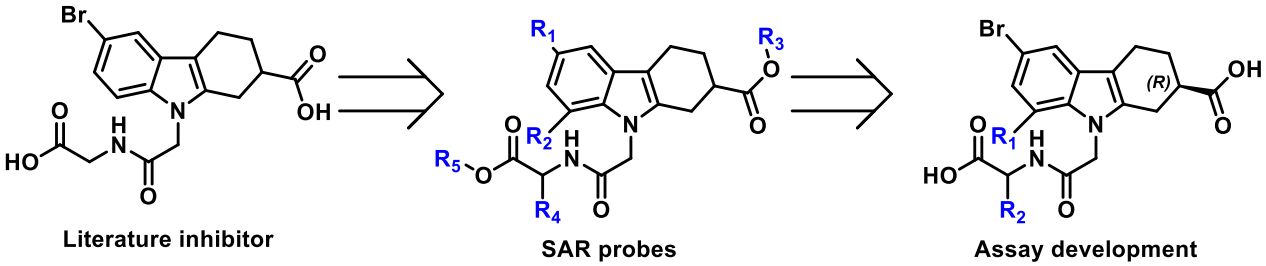
The β sliding clamp is an emerging antibiotic target that increases the transcription rate and processivity of the bacterial replisome[1]. Blocking the protein-interaction interface with small molecules should prevent the protein from interacting with polymerases, leading to SOS response and eventually to cell death. We have synthesized a series of racemic tetrahydrocarbazoles based on a literature inhibitor[2] that probe this binding pocket and have tested them towards the *E.coli* β-clamp using saturation transfer difference NMR-based assay. To obtaine binders with higher activity enantiopure derivatives were synthesized starting with a classical resolution. Although, binding to the *b*-clamp is confirmed, the compounds have low activity in culture, possibly due to poor cell wall penetration. Instead, the fluoro-containing compounds prepared are now evaluated as probes in NMR-based screening methods for identifying new β-clamp inhibitors.



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Unleashing the Potential of Therapeutics: The Promise of Monodisperse PEGs

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Polyethylene glycol (PEG) stands as the premier biocompatible polymer extensively employed in medical applications. Its usage spans across a wide spectrum of pharmaceutical products, including oral drugs, topical medications, and most prominently, in the COVID-19 vaccines. Industrially produced PEG typically exhibits polydispersity, consisting of PEG chains with at least 10 different lengths. Conversely, monodisperse (or uniform) PEGs comprise a single PEG chain length, albeit they are less common and available in smaller quantities at a higher cost.[1, 2]

Our objective in this study was to pioneer methods for producing monodisperse PEG derivatives essential to the pharmaceutical industry. Specifically, we aimed to establish pathways for synthesizing in-demand monodisperse PEG-lipids, such as DMG-PEG 2000, utilized in the Moderna COVID-19 vaccine.[3] Additionally, we aimed to create a diverse repository of PEG-peptides, evaluating them as potential candidates for pancreatic cancer vaccines.

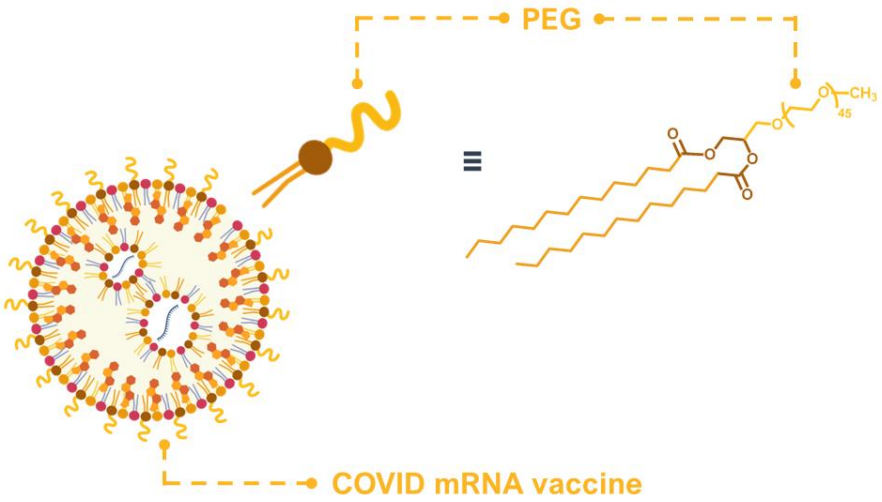

Figure 1. *PEG in the COVID-19 (Moderna) vaccine structure.*

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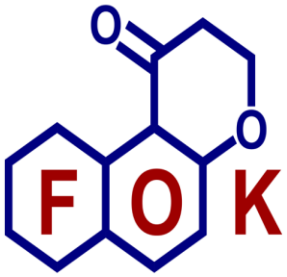

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Synthesis of a linker for incorporation into a MOF structure

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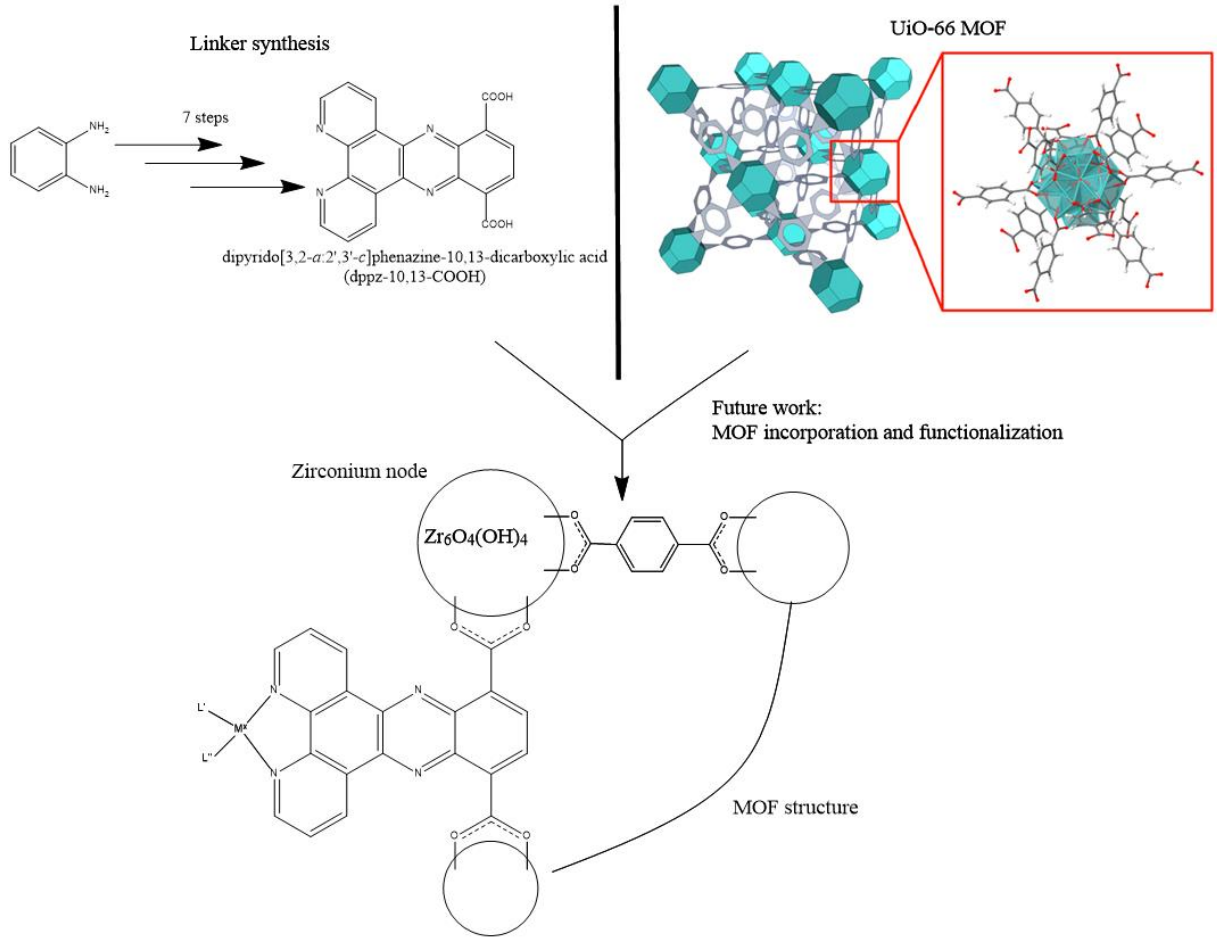
The linker is to be incorporated into a MOF structure. Following this, copper will be introduced to create a homogenous photoactive complex for catalysis.

The first stage of this project; the synthesis of the linker 10,13-dicarboxylic acid substituted dppz (dppz = dipyrido[3,2-a:2',3'-c]phenazine) is presented. Synthesis of UiO-66 MOF and characterization by powder X-ray diffraction, N_2 adsorption/desorption isotherms and thermogravimetric analysis is also presented.

Future work will include incorporation of the linker into a MOF structure, complexing with copper and possibly testing for catalytic activity towards CO_2 activation.



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Synthesis studies towards novel FMN riboswitch ligands

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The global health issue regarding antibiotic resistance bacteria is a pressing matter. The number of deaths caused by diseases previously treated with antibiotic is rising, estimating that it could cause 10 million deaths each year by 2050. Therefore, the discovery of new antibiotics to supress this trend is of high importance. [1-3]

Riboswitches are emerging as promising targets for developing a new type of antibiotics. These non-coding mRNA elements can assume different conformations that act as genetic switches, allowing them to control translation and transcription processes. These will then affect the production and expression of enzymes related with the synthesis of metabolites crucial for the bacteria's survival. In addition, these mRNA elements are mostly present in bacteria, which makes them good targets for the development of novel antibiotics. Riboswitches have two domains: an aptamer domain and an expression platform. The natural ligand binds in the aptamer domain leading to a conformational change and, consequently, induces the expression platform to translate it into expression or repression of the downstream genes. [1-3]

In this project, the flavin mononucleotide (FMN) riboswitch is of particular interest, being our main target for the development of new potential antibiotics. Through a virtual screening study, several promising ligands have been identified. Our work toward synthesis of a small library of analogues will be presented.

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Synthetic studies towards amphipathic pyrazino-pyrimidine-dione scaffolds for antimicrobial testing

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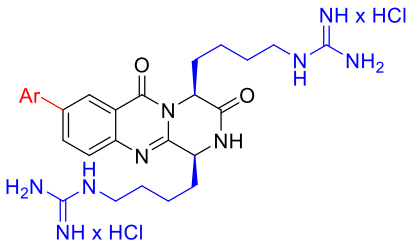
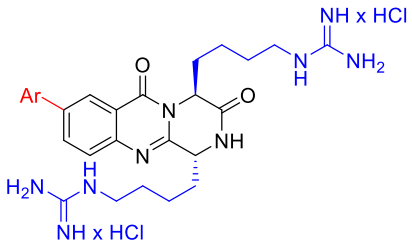
Antimicrobial resistance is one of the fastest growing medical issues of our generation.[1,2] To combat this, novel antibiotic compounds must be prepared. Inspired by antimicrobial marine peptides (AMP)[3,4] and amphipathic barbiturates[5], a series of new target molecules, (*S,S*)-**T** and (*S,R*)-**T**, are proposed. Ar = aryl.

The poster will show our latest synthetic work towards (*S,S*)-**T** and (*S,R*)-**T** based on start materials (*S*)-**1**, (*R*)-**1** and **2.**

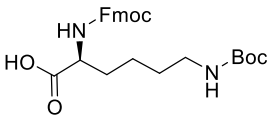


(*S,S*)-**T**

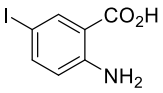


(*S,R*)-**T**

Start materials:



(*S*)-**1**



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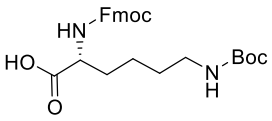

(*R*)-**1**

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Synthetic Studies Towards RvD1$_{n\text{-}3\ DPA}$ Analogs

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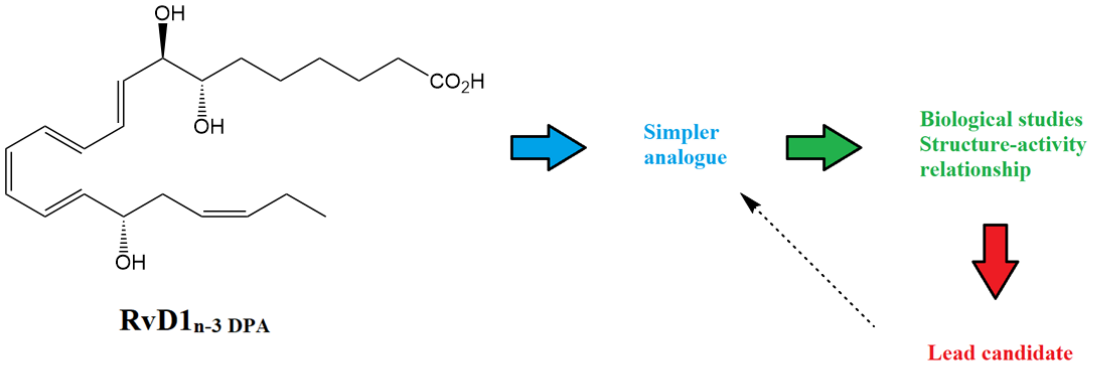
Specialized pro-resolving lipid mediators (SPMs) are biosynthesized from n-6 and n-3 polyunsaturated fatty acids during the resolution phase of an acute inflammation.[1] In 2013, the SPM RvD1$_{n\text{-}3\ DPA}$ was reported[2] and is an excellent biotemplate for the development of new, small molecular anti-inflammatory drugs and immunoresolvents.[3] Such simpler analogues are currently in development in our group based on the total synthesis of RvD1$_{n\text{-}3\ DPA}$.[4]



In this poster, we will present our initial synthetic efforts.

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Renewable phosphine ligands for homogeneous catalysis

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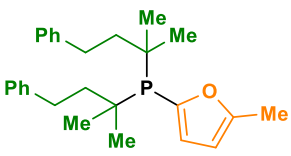
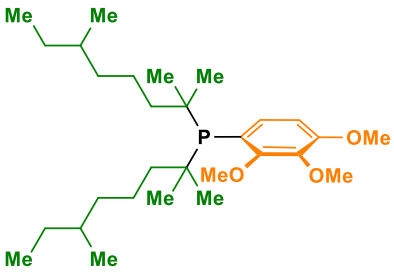
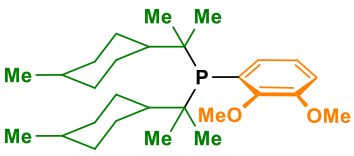
In the pursuit of sustainable catalysis, homogeneous catalysis featuring first-row transition metals has emerged as a prominent avenue. Despite inherent challenges in recycling and reusability, the reliability and comprehensive understanding of the mechanisms underlying homogeneous catalysts make them a compelling choice. Contemporary catalysts employed in organic synthesis often comprise a combination of metals and ligands, necessitating a holistic approach to sustainability that extends to both the metal and the ligand.
This presentation delves into the quest for a truly sustainable homogeneous catalyst, wherein the ligand is sourced from renewable building blocks. Recent investigations have illuminated the potential of biomass-derived molecules as viable precursors for crafting renewable analogues of well-established phosphine ligands, such as those pioneered by Beller.[1]
To address the stereoelectronic requirements crucial for effective phosphine tuning, we have introduced renewable analogues of Stradiotto's phosphine ligands.[2] These analogues are characterized by di-tertiary alkyl substituents and an aryl moiety and are derived from renewable starting materials. Our ligands exhibit efficacy in Pd-catalyzed Suzuki-Miyaura and Buchwald-Hartwig coupling reactions, achieving high yields. This multifaceted approach to sustainable homogeneous catalysis represents a significant stride towards greener synthetic methodologies.



From Papaya isobutyrate and 2-Methylfuran



From Dihydromyrcenol and Pyrogallol



From (−)−α-Terpineol and Guaiacol

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Synthesis and crystal structure of *N,N'*-disubstituted guanidines

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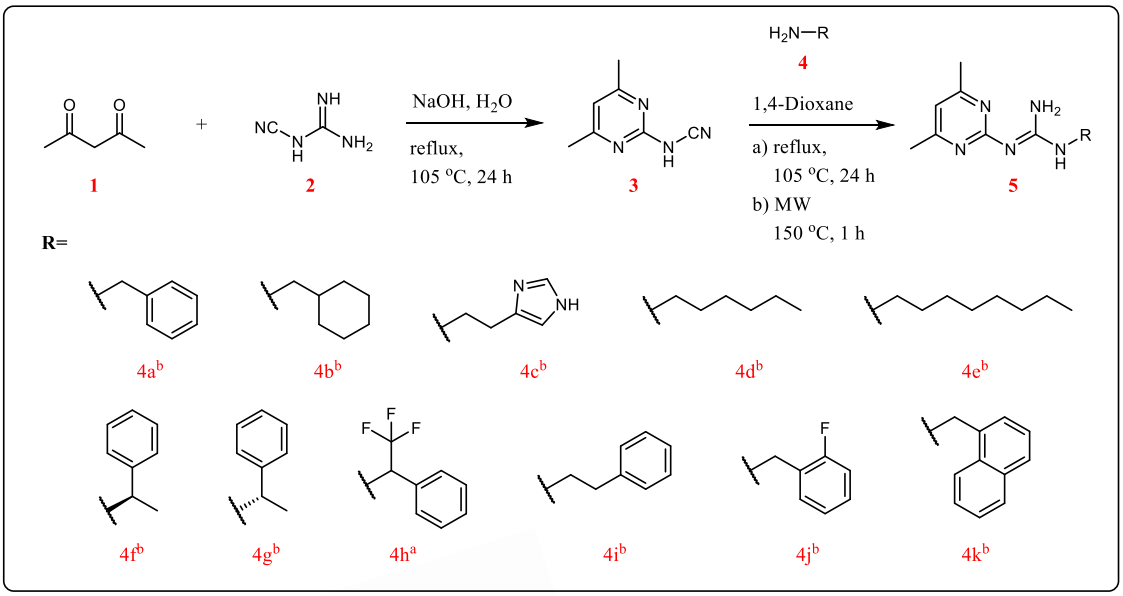
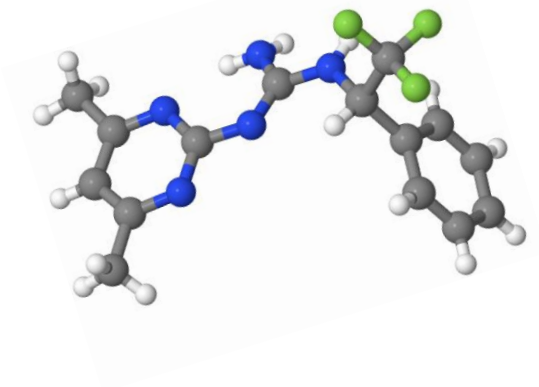
Guanidine and derivatives have piqued the interest of medicinal chemists for decades[1], and guanidine-based structures show a range of bioactivities including among others malaria[2] and tuberculosis[3]. In a library screening for activity towards DNA glycosidases (ca. 70 000 compounds), a disubstituted guanidines was identified as a potential inhibitor. Thus, we needed a range of guanidines for structure-activity studies. This work has focused on pyrimidine containing guanidines flanked by benzylic and aliphatic amines. The poster presents synthesis of the cyanamide **3**, tuning of the amination using benzylamine as a model compound, and the crystal structures of three new *N,N'*-disubstituted guanidines.





Crystal structure of 5h

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Green synthesis of ormeloxifene: A selective estrogen receptor modulator

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Ormeloxifene is the only birth control pill that is non-hormonal, which means it exhibits almost none of the side effects commonly associated with other contraceptives. As part of a novel pathway to ormeloxifene, methyl 4-hydroxycinnamate was exposed to tert-butyldimethylsilyl chloride, triethylamine and DMAP in dry THF to give methyl (*E*)-3-(4-((tert-butyldimethylsilyl)oxy)phenyl)acrylate in 90% yield, which then underwent a Grignard reaction in dry diethyl ether under inert conditions using methylmagnesium bromide to give (*E*)-4-(4-((tert-butyldimethylsilyl)oxy)phenyl)-2-methylbut-3-en-2-ol in 87% yield. The protection group was then removed by dissolving in a dimethylformamide:water mixture and reacting with cesium carbonate to give 4-[(1*E*)-3-hydroxy-3-methylbut-1-en-1-yl]phenol in 90% yield. The overall yield was 70% and 4-[(1*E*)-3-hydroxy-3-methylbut-1-en-1-yl]phenol was obtained in >99% purity. 4-[(1*E*)-3-Hydroxy-3-methylbut-1-en-1-yl]phenol is an aryl allyl alcohol, meaning it has great potential as a future precursor to pharmaceutical compounds.

Tetrasubstituted hydantoins: Novel membranolytic antimicrobials

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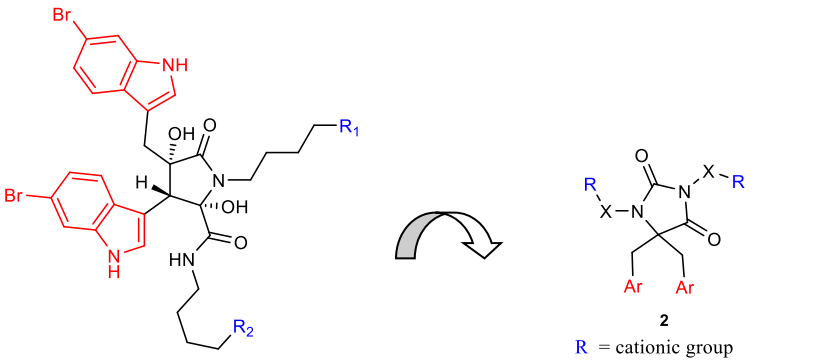
Antimicrobial resistance (AMR) among bacteria is getting evermore prominent and infections linked to AMR bacteria have a projected death toll of 10 million by year 2050.[a] In the search for new potential antimicrobials, marine isolates are a rich and largely untapped source of molecular scaffolds. In 2009 and 2011 a group of molecules called the eusynstyelamides (**1**) were isolated from the Australian ascidian *Eusynstyela latericius* and the Arctic bryozoan *Tegella cf. Spitzbergensis*, respectively. These molecules exhibited moderate antimicrobial activity.[b],[c] They consist of a five-membered dihydroxybutyrolactam ring substituted with two lipophilic groups and two cationic groups (amine or guanidine). Their mode of action (MoA) was assumed to primarily target and disrupt the bacterial membrane due to their amphipathic nature.



Eusynstyelamide (**1**)
R_1 = amine, guanidine
R_2 = amine, guanidine

R = cationic group
X = hydrophobic linker
Ar = (subst.) aryl, heteroaryl

Starting from the eusynstyelamides, we have simplified the core structure to a hydantoin motif and have synthesized a number of tetrasubstituted hydantoins **2** with improved potency while keeping the amphipathic properties unchanged. We have further investigated the MoA and potential synergistic effects of our newly synthesized compounds.

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Synthetic Studies Towards $RvD1_{n\text{-}3\ DPA}$ Analogs

Jonathan Büsser, Amalie F. Reinertsen and Trond V. Hansen

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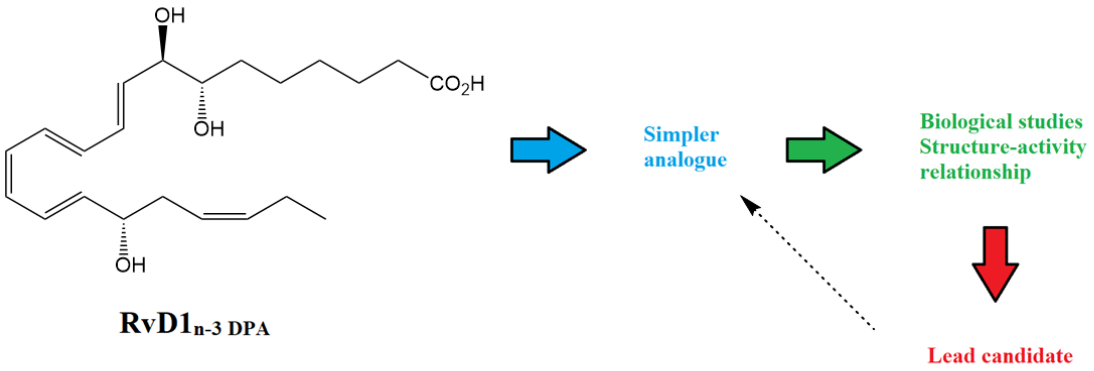
During the resolution phase of an acute inflammation, n-3 polyunsaturated fatty acids are used to biosynthesize specialized pro-resolving lipid mediators (SPMs).[1] The synthesis of new SPMs is of great interest as, unlike conventional drugs, they are capable of dampening inflammation processes without causing negative side effects such as interfering with the immune response.[2,3]

In 2013, the SPM $RvD1_{n\text{-}3\ DPA}$ was reported[4] and is an excellent biotemplate for the development of new, small molecular anti-inflammatory drugs and immunoresolvents.[5] Such simpler analogues are currently in development in our group based on the total synthesis of $RvD1_{n\text{-}3\ DPA}$.[3]

In this poster, we will present our initial synthetic efforts.



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Synthetic studies towards Dysoxylactam A

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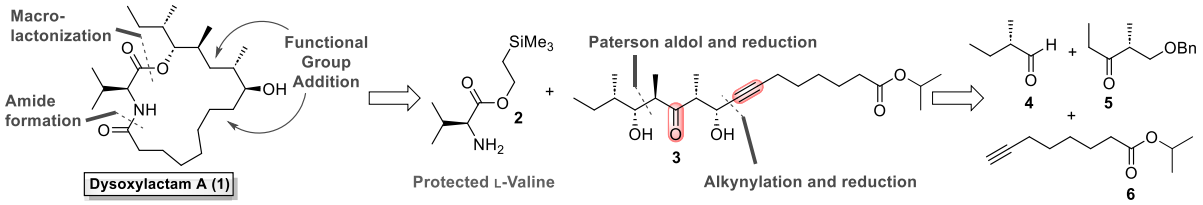
Recently the natural product dysoxylactam A (**1**, dA) was reported.[1] It was isolated from *Dysoxylum hongkongense* and preliminary data demonstrated the compound to be an effective and potent inhibitor of P-gp function in a Rho-123 accumulation assay. In MCF7/ADR cells, dA significantly increased intracellular accumulation of Rho-123, similar to the classical inhibitor of P-gp transporter verapamil. The dose-dependent behavior in which the natural product functions will be confirmed by flow cytometry analysis, and the compound was shown to decrease adriamycin efflux. dA did not significantly alter the expression of P-gp protein in all tested multidrug-resistant cell lines. Taken together, these results indicate that dA inhibits P-gp transporter function, and has the ability to significantly restore the sensitivity of P-gp-substrate drugs like adriamycin, vincristine and paclitaxel in drug resistant cancer cells.[1]

The retrosynthetic analysis shown below illustrates the chosen disconnections of dA (**1**), which resulted in four fragments of similar size. Our progress towards realizing an efficient synthesis of dA will be presented.



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Bioinspired copper complexes for selective methane oxidation and their incorporation into UiO-67

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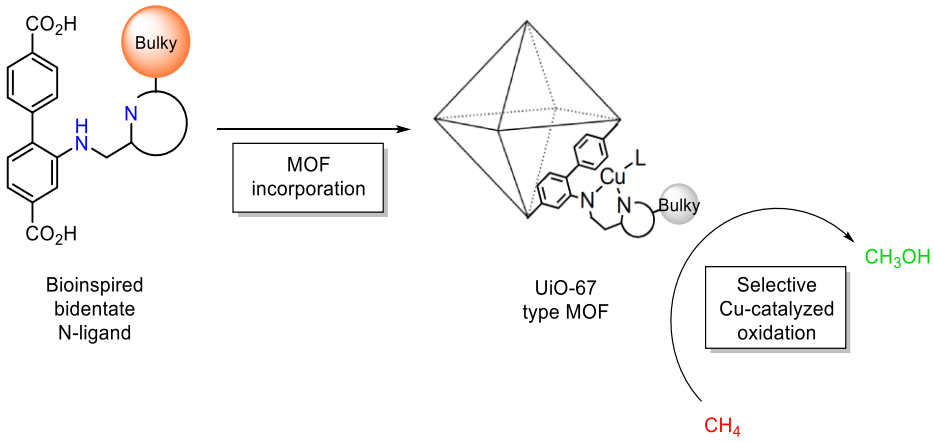
Selective oxidation of methane to methanol continues to be a challenge within the field of C—H activation.[1] However, nature can be used as inspiration; particulate methane mono-oxygenase (pMMO) and lytic polysaccharide monooxygenase (LPMO) are two examples of enzymes utilizing N-ligated copper as the cofactor to selectively oxidize C—H-bonds to alcohols.[2,3] Recent efforts have been directed towards integrating catalytic copper complexes inspired by these monooxygenases into UiO-67 type metal-organic frameworks (MOFs).[4,5] Thus far, the copper complexes bearing tri- and tetradentate N-ligands have been the focal point of the research;[4,5] therefore, this work explores the less studied counterparts bearing bidentate N-ligands. However, since opening more coordination sites can destabilize the copper complex, the effect of installing a bulky group on the N-ligands in order to counteract the destabilization is also investigated. Reactions such as reductive amination, the Suzuki-Miyaura coupling and ester hydrolysis are used in the linker synthesis. The MOFs are characterized using XRD, TGA, N_2-absorption and liquid phase digestion ^{1}H NMR.



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Synthesis of carbazole derivatives for testing as antibacterial agents

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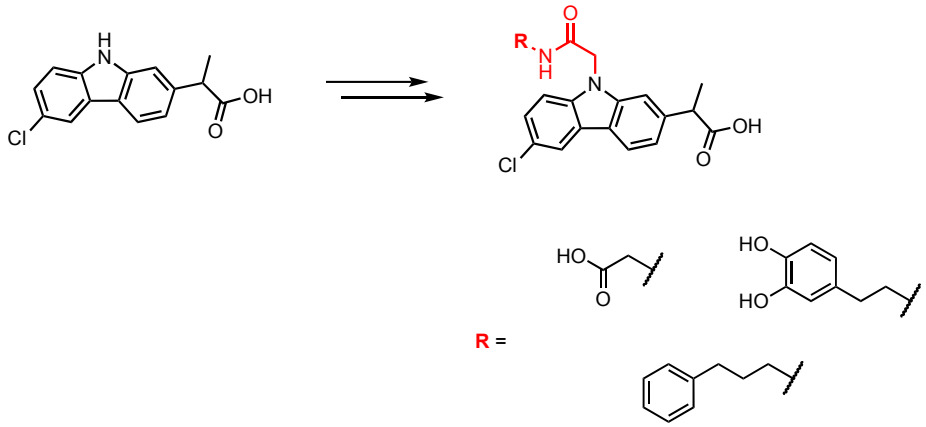
The bacterial DNA sliding clamp, called β-clamp, is one of the key proteins involved in DNA replication. The clamp encircles DNA and increases the rate of polymerase processivity.[1] An inhibition of the clamp will inhibit DNA replication, induce SOS response and potentially lead to cell death. Carbazoles are important scaffolds in drug development and are utilized in several anti-inflammatory agents.[2] Yin. et al have proved that such structures could bind to the β-clamp and be potential guides to new antibacterial agents.[3] An issue with these compounds is that they have limited cell activity. A potential way into the cell can be through the iron transport system. This may be achieved by including structural elements that are common in naturally occurring iron-chelating sideophores, such as catechols.[4]

This poster presents our work towards new carbazole derivatives, including a compound with a catechol-containing dopamine sidechain. In a central amide coupling step, different coupling reagents have been tested and evaluated in terms of efficiency, hazards and costs.



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Synthesis of an π-extended electron-donating unit suitable for n-type semiconductor in bulk-heterojunction solar cell

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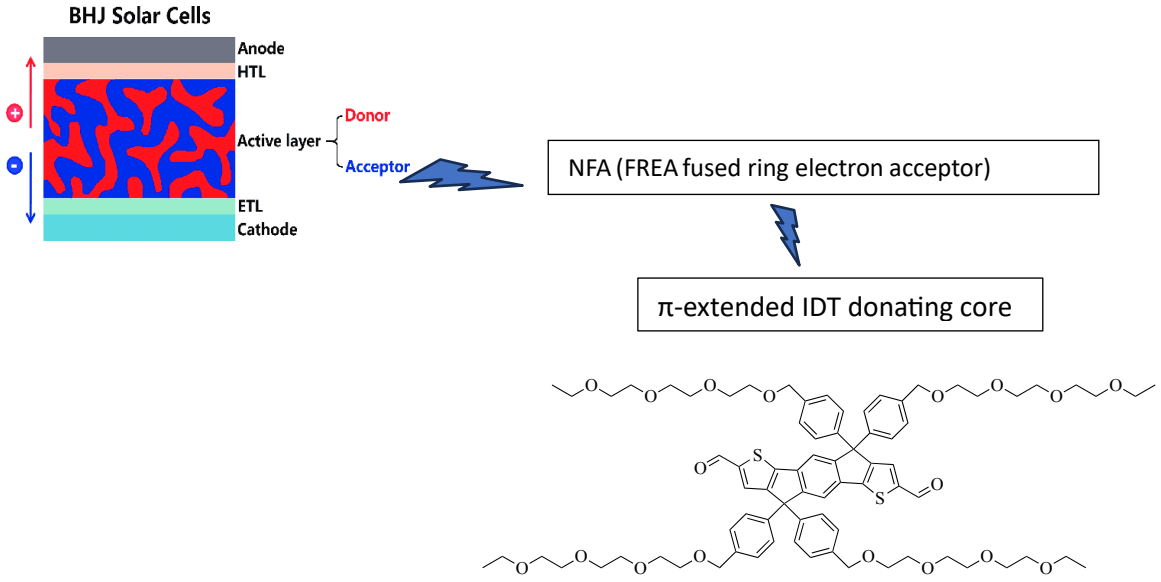
Organic solar cells (OSCs) based on the bulk-heterojunction (BHJ) have attracted attention in photovoltaic technologies for solar energy because of their flexibility, stretchability, and the possibility to be integrated into many diverse materials. (1) BHJs typically exhibit a "sandwich" configuration, wherein the photoactive layer comprises an electron donor material, often a conjugated organic polymer serving as the p-type semiconductor, and an electron acceptor small molecule (SMA) acting as the n-type semiconductor. These layers are enclosed between two interlayers, an electron-transporting layer (ETL) and a hole-transporting layer (HTL). (2) Lately, there has been a shift in attention towards the advancement of n-type semiconductors in organic solar cells, with a focus on non-fullerene electron acceptors (NFAs). The significant progress in organic solar cells containing NFAs is often related to the category of fused-ring electron acceptors(FREAs). FREAs are precisely defined organic compounds that exhibit a push–pull architecture, wherein π-extended donating cores, featuring four or more aromatic fused rings, are situated between two electron-withdrawing units (A-D-A or A-D-A-D-A-D-A). Here, A represents the electron-withdrawing group, and D represents the electron-donating group. (3) In this study, a π- π-extended donating core (IDT core group), specifically belonging to the IDIC family, is synthesized. The goal is to couple this donating group to electron withdrawing units which are synthesizing in parallel and yields an n-type semiconductor polymer or small molecule. the graphical abstract is shown below.



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Synthetic Studies Towards Fuligopyrone B

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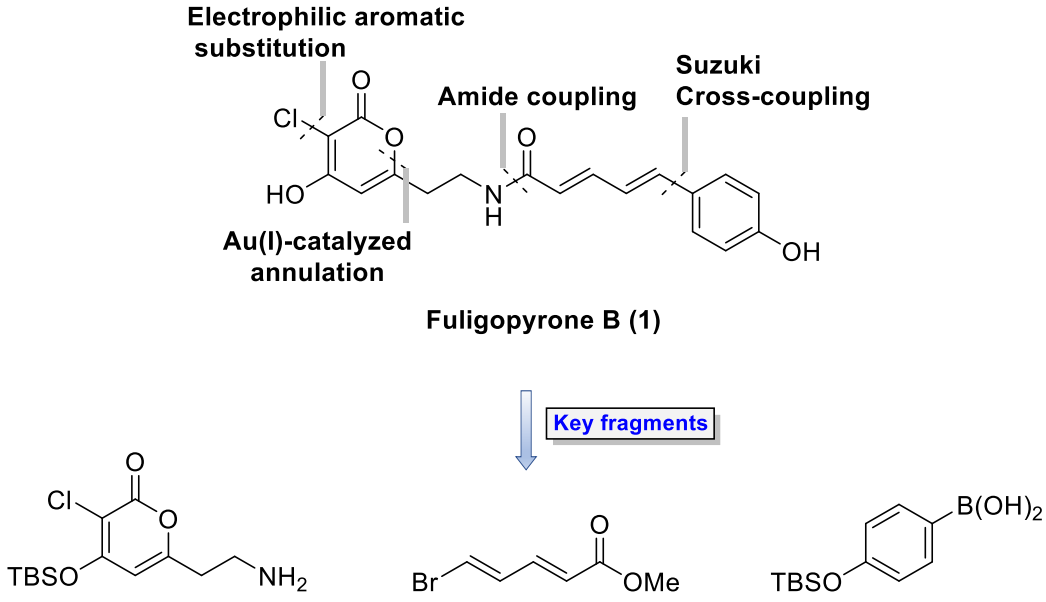
Fuligo septica is a yellow slime fungus that belongs to the class myxomycetes,[1] and has been a source for several aromatic yellow pigments with antibiotic activity.[2] Fuligopyrone B (**1**) was isolated from the above-mentioned fungus in 2023.[3]

Structurally, fuligopyrone B (**1**) contains a chlorinated α-pyrone moiety, and there are few reported synthetic methods for the introduction of chlorine to the pyrone nucleus in high yields. This part of the synthesis thus became an area of high focus. Our progress towards realizing an efficient synthesis of fuligopyrone B (**1**) will be presented.



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Synthesis of an electron donating unit suitable for n-type semiconductor in biosensor application

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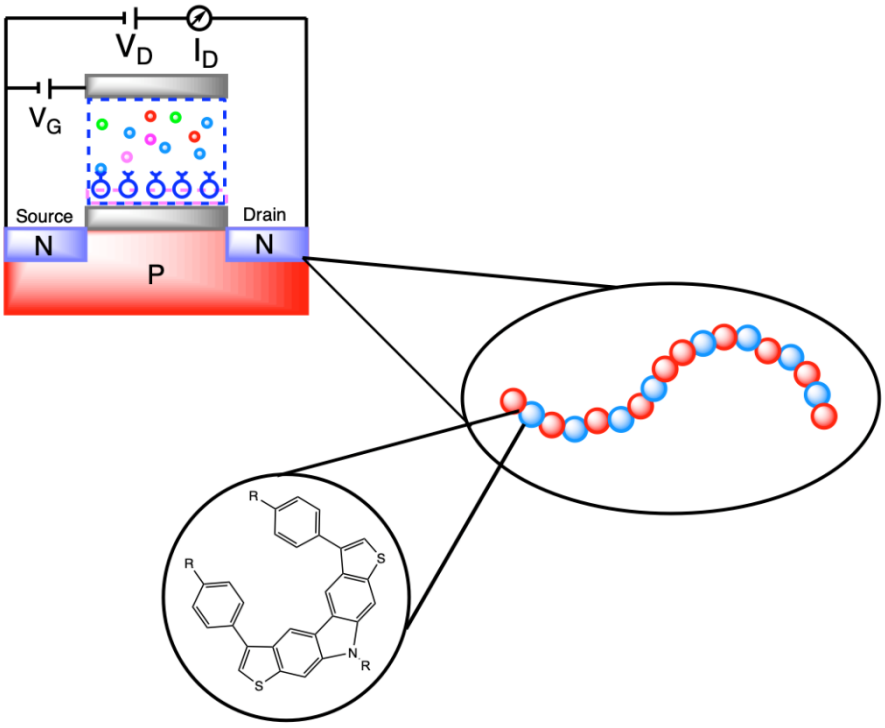
Advances within biotechnology and the need for rapid diagnosis to alleviate the need for precious time and expertise has resulted in a renewed interest in biosensor technologies. Organic biosensors has multiple important advantages, being made from cheap raw materials, possibility for flexible design, and possibility to adjust towards almost any biological recognition element.[1] Organic biosensors are essentially electrochemical field effect transistors (OEFTs) and thus, require high performing p-type and n-type materials. In the field of organic electronics there appears to be an overabundance of high performing p-type materials but a limited amount for n-type. This also holds true for OEFTs which require some additional characteristics like increased hydrophilicity and biocompatibility. In this work, a fused aromatic electron donor unitis synthesized based on the well-known carbazole moiety. Fused aromatics have shown advantages as weak-electron donor units in high performing organic optoelectonics.[2][3] The goal is to decorate this chromophore with glycol chains and subsequently couple it with a variety of strong electron acceptor units, synthesized in parallel, and yield an n-type semiconductor polymer or small molecule. The product will be evaluated in an OFET biosensor device. A graphical abstract is given below, which illustrates where in the OFET application an electron donating unit will be placed in an n-type semiconductor material.



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Benzothiadiazole-based acceptor moieties for semiconductors

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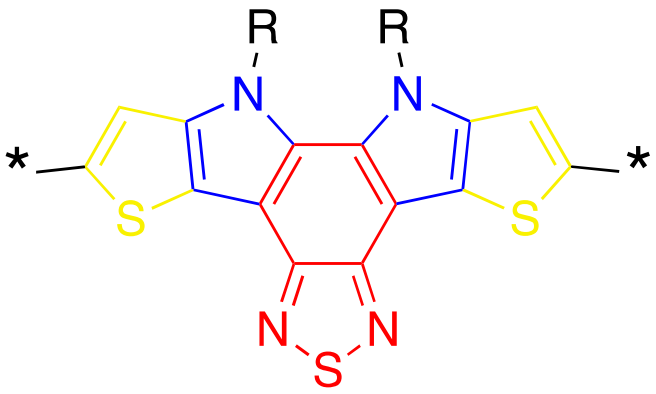
The demand for high-performance semiconductors in various applications has prompted a focus on developing novel molecular architectures. This project centers around the synthesis of fused aromatic acceptor molecules derived from the benzothiadiazole (BT) moiety. Benzothiadiazole, known for its electron-accepting properties, serves as a versatile building block for constructing semiconductor materials with enhanced electronic characteristics[1]. Coupled with an electron-rich donor, the electron deficient BT can be used to build a low band gap polymer.

In this project the electron-accepting BT moiety is covalently coupled with thienyl rings or pyrene moieties in a locked planar conformation. Our approach involves the modification of benzothiadiazole through tailored synthetic routes, aiming to create a diverse array of acceptor moieties. By introducing specific functional groups and tuning the molecular structure, we seek to optimize the electronic properties of the resulting molecules for semiconductor applications. These acceptor moieties hold great potential for integration into various organic electronic devices, such as organic electrochemical transistors (OECTs) which are used as biosensors. Suitable flexible chains will be incorporated on the end-product to promote solubility in common organic solvents for the desired biocompatibility.



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Investigations into copper-catalyzed *N*-alkynylation of hydantoins: A strategy for further functionalization.

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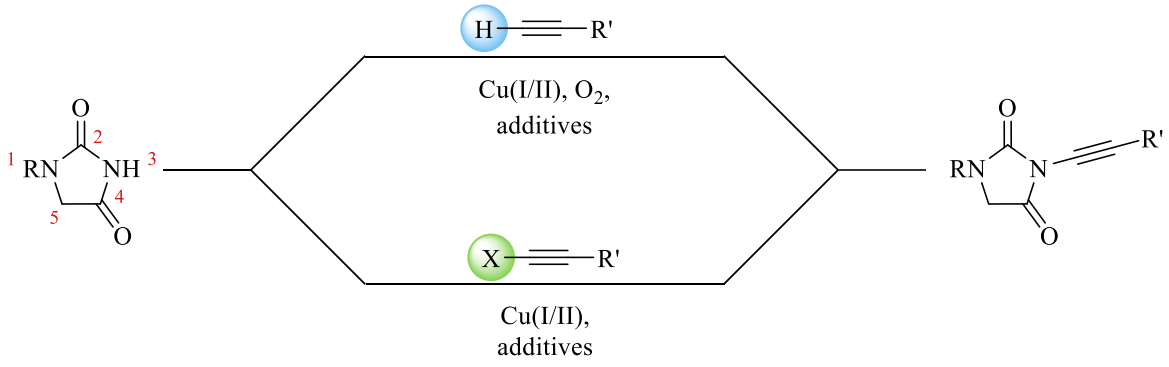
Hydantoin and its derivatives are known for a large number of different biological activities and is used in medicinal as well as agrochemical applications.[1] The classical methods for synthesizing various hydantoins involve functionalization of linear precursors with a cyclization reaction as the final step. These cyclization methods are usually based on toxic reagents and harsh conditions. Therefore, the investigations into new synthetic strategies for modifying hydantoins directly and selectively on N-1, N-3, and C-5 are of general interest.[2]

This project is focused on developing a general method for the direct N-3- and/or N-1-alkynylation of different hydantoins. A direct and reliable synthesis for these nitrogen-substituted alkynes, so-called ynimides and ynamides, opens various possibilities for further functionalizations.[3] Moreover, the alkynylhydantoin moiety itself is poorly described in literature.

Copper has an important role in catalyzing the formation of C-N bonds. Its high tolerance towards other functional groups and its strong tendency to coordinate both heteroatoms and π-systems makes it ideal for investigating *N*-alkynylations. Therefore, the reactivity of hydantoins in different Cu-catalyzed cross-coupling with alkynes has been explored. Both haloalkynes and terminal alkynes have been tested as alkyne substrates, the latter of which requiring oxidative conditions.[4,5]



R = H, CH_3 ; R' = Alk, Ar ; X = Hal

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Synthesis of *N*-1-arylhydantoins through an enimide protection strategy

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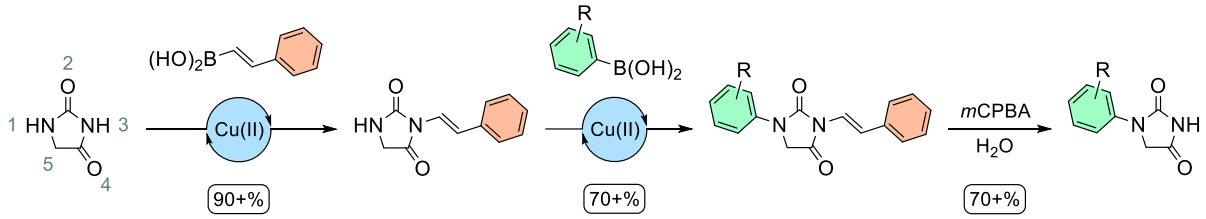
Hydantoin is a heterocyclic scaffold found in a large variety of structures across different fields, including pharmaceutical chemistry, agricultural sciences, water treatment and semiconductor technology. The usual synthetic route for producing substituted hydantoins is through cyclisation of a functionalised acyclic precursor, for which toxic reagents and harsh conditions are often necessary. [1] This approach can be limiting for potential retrosyntheses, thus making the development of new direct functionalisation methods interesting to pursue.

Achieving direct functionalisation at the N-1 position has the added challenge of it typically being less reactive than the more acidic N-3 position. In the case of direct *N*-1-arylation, the only existing generalised method requires a prefunctionalised N-3 position. [2] Protection of N-3 seems like an apparent solution, yet no synthesis of *N*-1-arylhydantoins *via* such a strategy has been reported. In fact, literature on the protection of hydantoin is scarce and sometimes contradictory, and yields often suffer from issues with regioselectivity. [3-4]



Herein we demonstrate the successful synthesis of different 1-arylhydantoins starting from the unsubstituted heterocycle, using (*E*)-2-phenylethenyl ("styryl") as a new protecting group. The work builds on a broad method for generating enimides previously developed in our group. [5] We show that the styryl motif is easier to attach than traditional protecting groups, and can be removed with less oxidising conditions than in reported enimide cleavage reactions. [6] Moreover, we describe an alternative *N*-1-arylation method based on a Cu-catalysed Chan-Lam cross-coupling reaction that is milder than previously reported methods.

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Synthesis and Reactivity of Imidazolyltetrazole Derivatives via Purine Ring Opening

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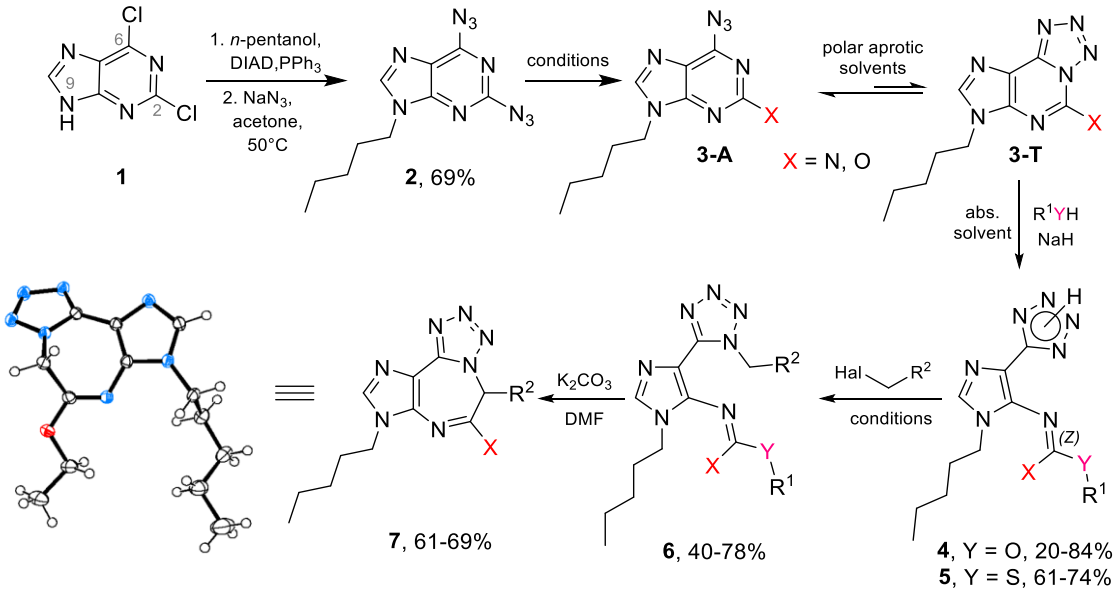
Imidazoles and tetrazoles are important pharmacophores with antibacterial and analgesic activities.[1] The present work focuses on S_NAr reactions of compound **3** with O- and S-nucleophiles. Compounds **3** exist in azido-tetrazole tautomeric equilibrium the extent of which is influenced by solvent, temperature and nearby electron-donating/electron-withdrawing groups.[2] The reactivity of ring opened products can further be explored by alkylating tetrazole ring and *in situ* creating tetrazolo fused 1,4-diazepine derivatives **7**.



Synthesis and reactivity of imidazolyltetrazole derivatives

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Synthetic efforts towards 4*S*,5*S*-dihydroxy docosapentaenoic acid

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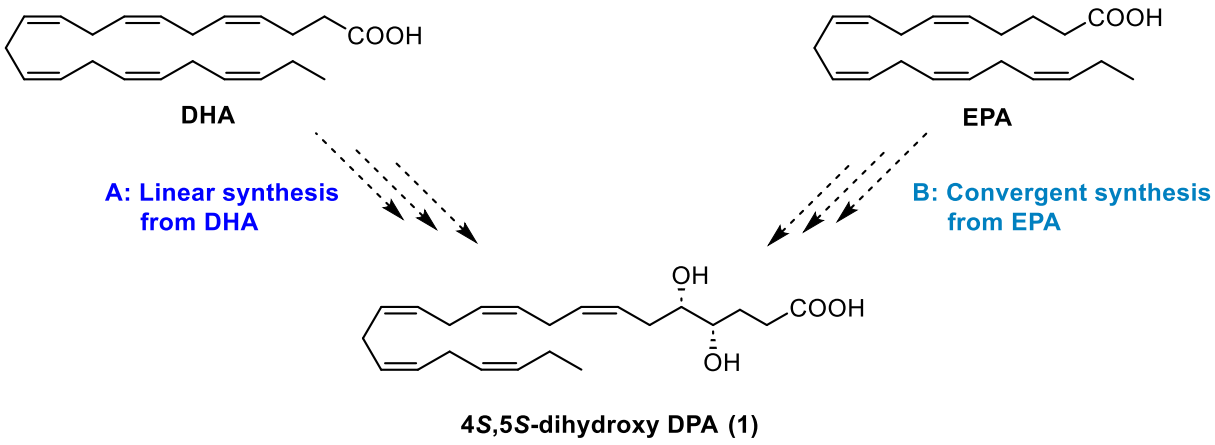
The polyunsaturated fatty acid (PUFA)-product 4*S*,5*S*-dihydroxy docosapentaenoic acid (DPA, **1**) has been isolated from various human samples[2] and is most likely enzymatically formed. This endogenous product has not yet been the target of a stereoselective total synthesis.

This poster presents some of the lessons learned during our attempted semi-synthesis of **1**, starting from commercially available docosahexaenoic acid (DHA) or eicosapentaenoic acid (EPA). This approach has successfully been used earlier for other PUFA-derived natural products.[2]



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Workshops

Saturday January 6th (10:30-12:00)

UiT Norges arktiske universitet

Building search strategies in Reaxys Academic Edition to tackle the Sustainable Development Goals (SDGs)

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As we take a closer look at ways to solve some of the pressing environmental and societal challenges of the current decade, we notice how the chemistry landscape yields itself to even more possibilities for positive change and innovation.[1] Chemists in all fields are well equipped to transpose approaches they commonly apply in their research to the advancement of the 17 Sustainable Development Goals of the United Nations General Assembly. In doing so, they can also rely on the power of available digital tools to build search strategies and queries designed to tackle one or more of the SDGs.

In this workshop, we will go through practical examples built using Reaxys Academic Edition, the leading digital tool for chemistry in academia, to approach different SDGs: zero hunger (SDG 2), clean water and sanitation (SDG 6), affordable and clean energy (SDG 7), among others. Once the SDG of interest is identified, we structure a tailored search in Reaxys to identify relevant literature, compounds of interest, their physicochemical and bioactivity properties, their commercial availability and synthesis, and any reported impact on biological targets. In addition, these examples will highlight advanced features that are part of Reaxys Academic Edition, including:

- the Retrosynthesis Planner, used to evaluate the relevance of all published synthetic routes for compounds of interest and to compare different synthetic approaches from reported procedures. Users can also easily customize synthetic routes by adding or removing reaction steps. In addition, the Planner is complemented by our AI-based Predictive Retrosynthesis feature that helps identify new possible, unpublished syntheses suggested by a 3N-MCTS algorithm, trained on over 15 M single-step reactions and 500'000 building blocks.[2]
- the Reaxys Target & Bioactivity insights, offering full access to a wide range of bioactivity data and critical parameters for hit-to-lead identification and lead optimization, and enables the investigation of biological targets in terms of the chemistry space: competitive landscape, structure-activity relationships, pharmacokinetic properties, toxicology/safety profiles.

Every chemist can use the information found in Reaxys Academic Edition to develop impactful research projects related to the advancement of the SDGs, for the benefit of our society and the environment.

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- *Introducing CAS life science content in SciFinder® that will permit medicinal chemists to evaluate drug-target-disease relationships.*

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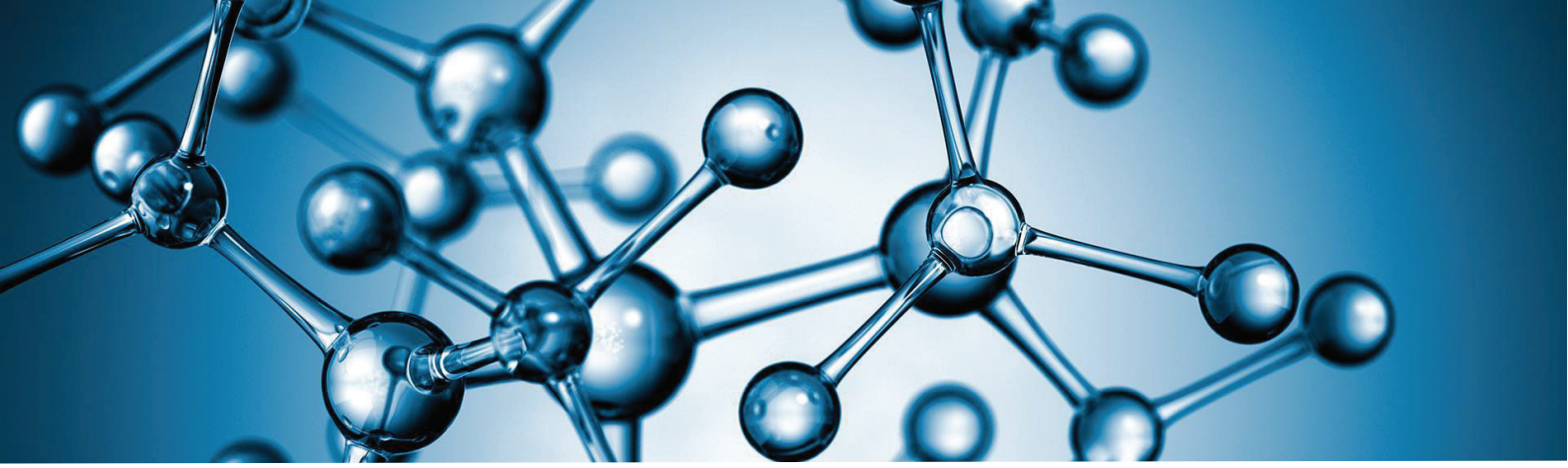

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