XII Young Investigator Workshop

Societat Catalana de Química (SCQ)

(Catalan Chemical Society),

EuChemS Divison of Organic Chemistry

Barcelona, 25th – 26th November 2021

EuChemS European Chemical Society — Division of Organic Chemistry —

SCQ Societat Catalana de Química

EuChemS

European Chemical Society

Division of Organic Chemistry

Prof. Gianluca Maria Farinola (President)

Prof. Anton Vidal (Chair of the YIW 2020)

Prof. Patrick Guiry (Incoming President)

Prof. Berit Olofsson (Secretary)

Prof. Michael Schnürch (Treasurer)

Prof. Wim De Borggraeve (Dissemination Officer)

Ass. Prof. José Luis Núñez-Rico (Organization Committee of the YIW 2020)

SCQ

Societat Catalana de Química

YIW 2020
XII Young Investigator Workshop

Contents

Welcome message from the Organizers

Dear participants, it is a great pleasure to welcome you in Barcelona for the 12th *Young Investigator Workshop* (YIW), the flagship event of the EuChemS Division of Organic Chemistry. The meeting has been jointly organized by the *Societat Catalana de Quimica* (SCQ) and the *EuChemS Division of Organic Chemistry* (EuChemS-DOC).

Following the concept and the tradition of our YIW, talented young researchers at the beginning of their scientific careers in organic chemistry from the EuChemS Organic Chemistry Division Member Societies meet, this time, in Barcelona on the 25th and 26th of November 2021, to present excellent research results.

It is specially exciting this time to reconvene together after more than a one-year break caused by the COVID-19 pandemic, and this is why this 2020 edition is being held in 2021. We are glad to have succeeded in maintaining our tradition to meet together in person– for most of the participants– ensuring the possibility to enjoy the scientific workshop and the social activities associated with it. The event will also host contributions from two YI representatives of the ACS, as well as from young researchers from industries and from chemistry journal editors, who have supported our workshop. We are grateful to the sponsors and to all the participants for their presence and contributions. We hope that, once again, our YIW will be a special occasion not only to share excellent research, but also to create networking and European identity in the organic chemists' community, which will last over the years.

We wish you an exciting 12th YIW and, once again, welcome to Barcelona!

Gianluca M. Farinola
President Divison of Organic Chemistry
EuChemS DOC

Anton Vidal
Chair of YIW 2020
Representative of the Catalan Chemical Society in EuChemS DOC

Berit Olofsson
Secretary Division of Organic Chemistry
EuChemS DOC

José Luis Núñez
Research Associate, University of Barcelona
Member of the Catalan Chemical Society

Institut d'Estudis Catalans (Institute for Catalan Studies, IEC) - site map of the event

The *Institut d'Estudis Catalans*, also known by the acronym IEC, is an academic institution which seeks to undertake research and study into "all elements of Catalan culture". The IEC is the Catalan academy of sciences and humanities and deals with all knowledge disciplines. It is based in Barcelona and located in the old "*Casa de Convalescència*" from the Old Hospital de la "*Santa Creu*", a 17th-century building.

(Pictures from IEC)

The EuCheMS YIW 2020 will take place at the *Institut d'Estudis Catalans* (Institute for Catalan Studies) in the Lecture Room "Pere i Joan Coromines" on the ground floor and at the right-hand side in the courtyard (see picture above), when entering the building. A map with the locations of the venue and the hotel is shown in the next page. The two closest underground stations to the venue and the hotel (from Line 2 and Line 3) are also indicated.

EuChemS DOC Members

Surname Name	Member Society/Supporting Member	Affiliation
Maulide Nuno	Gesellschaft Österreichischer Chemiker (GÖCH) – Austrian Chemical Society	University of Vienna
De Borggraeve Wim	Société Royale de Chimie (SRC) – Walloon Royal Society of Chemistry. Koninklijke Vlaamse Chemische Vereniging (KVCV) – Royal Flemish Chemical Society	KU Leuven
Roje Marin	Hrvatsko kemijsko društvo (HKD) – Croatian Chemical Society	Rudjer Boskovic Institute
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Kotora Martin	Ceská spolecnost Chemická (CSC) – Czech Chemical Society	Charles University
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Gathergood Nicholas	Eesti Keemia Selts (EKS) – Estonian Chemical Society	Tallinn University of Technology
Koskinen Ari M.P.	Suomalaisten Kemistien Seura (SKS) – Finnish Chemical Society	Aalto University
Vidal Virginie	Société Chimique de France (SCF) – French Chemical Society	Ecole Nationale Superieure de Chimie de Paris
Bräse Stefan	Gesellschaft Deutscher Chemiker (GDCh) – German Chemical Society	Karlsruhe Institute of Technology (KIT)
Kokotos Christoforos	Ένωση Ελλήνων Χημικών – Association of Greek Chemists (AGC)	University of Athens
Kurtán Tibor	Magyar Kémikusok Egyesülete (MKE) – Hungarian Chemical Society	University of Debrecen
Guiry Pat	Institúid Ceimice na Héireann – Institute of Chemistry of Ireland (ICI)	University College Dublin
Marek Ilan	החברה הישראלית לכימיה – Israel Chemical Society	Israel Institute of Technology, Technion
Farinola Gianluca	Società Chimica Italiana (SCI) – Italian Chemical Society	University of Bari “Aldo Moro”
Butkus Eugenijus	Lithuanian Chemical Society	Vilnius University
Jirgensons Aigars	Latvijas Zinātņu akadēmija – Latvian Academy of Sciences	Riga Technical University

Minnaard Adriaan	Koninklijke Nederlandse Chemische Vereniging (KNCV) – Royal Netherlands Chemical Society	University of Groningen
Haug Bengt Erik	Norsk Kjemisk Selskap (NKS) – Norwegian Chemical Society	University of Bergen
Mlynarski Jacek	Polskie Towarzystwo Chemiczne (PTC) – Polish Chemical Society	Polish Academy of Sciences, Warsaw
Silva Artur	Sociedade Portuguesa de Química (SPQ) – Portuguese Chemical Society	University of Aveiro
Egorov Mikhail	Российское химическое общество им. Д.И. Менделеева – Mendeleev Russian Chemical Society (MRCS)	Russian Academy of Sciences
Opsenica Igor	Српско хемијско друштво (СХД) – Srpsko hemijsko društvo (SHD) – Serbian Chemical Society	University of Belgrade
Jakubec Pavol	Slovenská chemická spolocnost (SCS) – Slovak Chemical Society	Slovak University of Technology in Bratislava
Mascareñas José Luis	Real Sociedad Española de Química (RSEQ) – Spanish Royal Society of Chemistry	University of Santiago de Compostela
Vidal Anton	Societat Catalana de Química (SCQ) – Catalan Chemical Society	ICREA and University of Barcelona
Olofsson Berit	Svenska Kemisamfundet – Swedish Chemical Society	Stockholm University
Bode Jeffrey W.	Société Suisse de Chemie – Schweizerische Chemische Gesellschaft – Swiss Chemical Society	ETH Zürich
Fuchter Matthew J.	Royal Society of Chemistry (RSC)	Imperial College London

Useful Information for Delegates

Workshop Venue

The EuCheMS YIW 2020 will take place in Lecture Room the Lecture Room "*Pere i Joan Coromines*" on the ground floor and at the right-hand side in the courtyard, when entering the building. A map with the locations of the venue and the hotel is shown in the next page. The two closest underground stations to the venue and the hotel (from Line 2 and Line 3) are also indicated.

Accommodation

Accommodation is booked for all delegates at Hotel Silken Ramblas (https://www.hoteles-silken.com/en/hotel-ramblas-barcelona/).
Pintor Fortuny, 13. 08001. Barcelona, Spain
T: +34 93 3 426 180 | F: +34 933 027 977
Coordinates:41°22'58.55''N / 2°10'12.24''E

The venue is within walking distance to the hotel.

Public Transportation

The event location is in a walking distance from Hotel Silken Ramblas Barcelona. The area is fully served with public transportation: Metro Lines L2 and L3 – See site map above.

The organizers suggest to have a look to the transportation network (https://www.tmb.cat/en/) to find the travel arrangements that better suits their plans.

As for the transportation from the airport to the hotel/venue, the **Aerobus** is a fast (35 minutes) shuttle bus that connects Barcelona airport (terminals T1 and T2) and the city centre. The closest bus stop to the hotel/venue from the Airport is "*Plaça Universitat*" (10-15 min walk to the the hotel/venue). The return bus stop (from the the hotel/venue to the Airport) is at the crossing of streets "*Sepúlveda*" and "*Urgell*". Please keep in mind that there are two lines (A1/A2), depending on your terminal (T1/T2 respectively). For more information, see:
https://www.barcelona.com/barcelona_city_guide/all_about/barcelona_airport_bcn/from_barcelona_airport_to_city_centre

The transportation from the airport to the hotel/venue is also possible with the underground. Take Line 9 (from terminals T1 or T2, orange line) and step down at "*Zona Universitària*". Catch then Line 3 (green line) to "*Liceu*", which is close to the venue/hotel (see map in page 8).

Additionally, the iconic black-yellow metropolitan cabs will be found all over the city and the airport.

Meals

Lunchs and Coffee breaks will take place in the courtyard of the *Institut de Estudis Catalans*.

Social dinner on Thursday 25th will take place at "*Restaurant Semproniana"* (https://semproniana.net/en/home/) – Carrer del Rosselló, 148, 08036 Barcelona.

Dinner on Friday 26th will take place at *the "Fàbrica Moritz"* (www.moritz.com) – Ronda Sant Antoni 39, 08011, Barcelona.

Presentations

Please upload your presentation at least 30 min before the start of the session that you are scheduled to speak in. For speakers delivering a lecture *via* the zoom platform, use the link that each speaker will receive nearer the time.

Badges & Security

For security purposes, all delegates and exhibitors MUST ensure they are wearing the YIW2020 badge at all times whilst on site.

Internet Access

Complimentary Wifi is available on site for the whole duration of the meeting.

Programme

Day 1: Thursday 25th November		
10:00 12:40 13:35	Registration Lunch (at IEC's courtyard) *Opening* (Profs. Messeguer (Board IEC), Farinola (President EuChemS DOC), Ujaque (President SCQ), Guiry (Incoming President EuChemS DOC) and Vidal (Chairman))	
	Session 1 – New Selective Methods in Organic Synthesis (Chairman: Gianluca M. Farinola)	
14:00	Davide Audisio	Sydnone-Based Approach to Heterohelicenes through 1,3-Dipolar-Cycloadditions
14:30	Janis Veliks	Sulfonium Reagents for Fluoromethylene Transfer Chemistry
15:00	Maria Koyioni	Synthesis of Canthin-4-one and Isocanthin-4-ones *via* B-Ring Construction
15:30	Søren Kramer	Catalytic Functionalization of C(SP^3)–H Bonds
16:00	Đani Škalamera	Efficient Synthesis of Linear Trisaccharide from QS-21
16:30	*Coffee Break*	
	Session 2 – Efficient Organic & Selective Transformations from the Industrial Point of View (Chairman: Anton Vidal)	
17:00	André Dieskau	How Modern Chemistry Contributes to Sustainability Objectives – Examples from Bayer AG Industrial speaker
17:35	Lucas Carreras	Homogeneous Catalysis in Organic Transformations – A View from Industry (Johnson Matthey) Industrial speaker
	Session 3 – Organic Synthesis for Bio-related Targets (Chairman: Patrick Guiry)	
18:10	Jakub Švenda	Reducing Synthetic Complexity of the Bactobolin Class of Ribosome Inhibitors
18:40	István Mándity	Development of Novel Continuous-Flow Synthesis Technologies and Utilization thereof in Peptide and Foldamer Chemistry
19:10	Elaine O'Reilly	Biocatalytic Approaches to Complex Targets
21:30	*Social Dinner at Restaurant Semproniana*	

Day 2: Friday 26th November		
	Session 4 – Light-Driven Synthetic Transformations (Chairman: Daniele Leonori)	
08:30	Luca Dell'Amico	Moving from Direct Photochemistry to Photoredox Catalysis - A Mechanistic Adventure
09:00	Maciej Giedyk	Photocatalytic Modifications of Organic Halides in Self-Assembled Aqueous Systems
09:30	Markus D. Kärkäs	Stereoselective Synthesis of Unnatural α-Amino Acids through Photoredox Catalysis
10:00	Shoubhik Das	Solar Energy Driven Sustainable Synthesis of Pharmaceuticals and Fuels
10:30	Jason P. Holland	Harnessing Photochemistry in Radiotracer Synthesis
11:00	*Coffee Break*	
	Session 5 – Supramolecular Chemistry – Spectroscopic Methods – Modeling (Chairwoman: Maria Koyioni)	
11:30	Bernd M. Schmidt	Fluorinated Porous Organic Cage Compounds
12:00	Maarten Smulders	Integrating the Hammett Equation into Covalent Adaptable Imine Networks
12:30	Boban D. Anđelković	FT-IR Spectroscopy as a Simple Tool for Rapid Solution of Various Problems
13:00	Jaime A. S. Coelho	Data-Driven Modeling of Bioorthogonal Reactions
13:30	*Lunch (Courtyard at IEC)*	

Programme

	Session 6 – New Selective Methods in Organic Synthesis - cont. (Chairman: Anton Vidal)	
14:30	Martín Fañanás-Mastral	Turning Simple Hydrocarbons into Multifunctional Building Blocks
15:00	Constantinos G. Neochoritis	A Multicomponent Tetrazolo Indole Synthesis
15:30	Ahmad Masarwa	α-*gem*-Diboryl Carbon-Centered Radicals: Towards Synthetic Diversity
16:00	Jørn E. Tungen	Stereoselective Synthesis of Specialized Pro-Resolving Lipid Mediators
16:30	Keary M. Engle	Catalytic Difunctionalization of Alkenes with Chiral Transient Directing Groups
17:00	*Coffee Break*	
	Session 7 – Electrochemistry in Organic Synthesis (Chairman: José Luis Núñez)	
17:30	David Cantillo	Sustainable Synthesis of Pharmaceutical Intermediates using Electrochemical Methods
18:00	Song Lin	Amping up Organic Synthesis with Electrochemistry
18:30	*Pause*	
	Session 8 – Sponships and YI Award of EuChemS Division of Organic Chemistry (Chairman: Michael Schnürch)	
18:45	Susanne Haak	The history of the relationship '*Thieme-YIW*'
18:55	Marta da Pian	A chemist in the library: the new research ecosystem
19:15	Daniele Leonori	New Methods in Halogen-Atom Transfer (XAT)
19:45	*YIW Award – Final remarks – Farewell* (Profs. Farinola (President EuChemS DOC), Marcé (Vice-President SCQ), Schnürch (Treasurer EuChemS DOC) and Vidal (Chairman))	
21:30	*Dinner at Fàbrica Moritz*	

List of Speakers and Abstracts

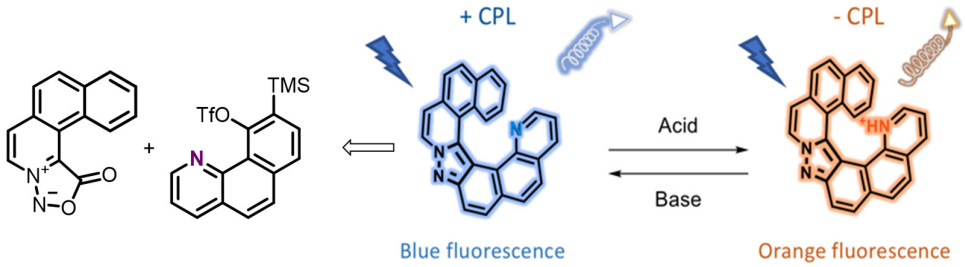
SYDNONE-BASED APPROACH TO HETEROHELICENES THROUGH 1,3-DIPOLAR-CYCLOADDITIONS

Expédite Yen-Pon,[a] Floris Buttard,[b] Lucas Frédéric,[a] Frédéric Taran,[a] Ken N. Houk,[c] Grégory Pieters,[a] Pier Alexandre Champagne,[b] Davide Audisio[a*]

[a] *Université Paris-Saclay, CEA, Service de Chimie Bio-organique et de Marquage, DMTS, Gif-sur-Yvette, France ;* [b] *Department of Chemistry and Environmental Science, NJIT, Newark, USA;* [c] *Department of Chemistry and Biochemistry, UCLA, USA.*

** e-mail: davide.audisio@cea.fr*

Despite their fascinating structures and unique properties, synthetic access to heterohelicenes remains challenging.[1] We reasoned that a late-stage formation of this helicoidal structure, through sydnone/aryne 1,3-dipolar cycloaddition, could allow a fast access to new polycyclic heteroaromatic hydrocarbons. This strategy would involve the key design of *ortho*-substituted polyaromatic sydnones. Over the process, an unprecedented regioselectivity in the cycloaddition step towards the more sterically constrained product was observed.[2] The origin of this observation was studied by DFT calculations and the chiroptical properties of the azahelicenes were investigated. This method allowed the divergent access to a variety of heterohelicenes and the characterization of a pH triggered chiroptical switch, with CPL-sign reversal.[3]



1. Dhbaibi, K.; Favereau, L.; Crassous, J. *Chem. Rev.* **2019,** *119*, 8846-8953.

2. Yen-Pon, E.; Champagne, P. A.; Plougastel, L.; Gabillet, S.; Thuéry, P.; Johnson, M.; Muller, G.; Pieters, G.; Taran, F.; Houk, K. N.; Audisio, D. *J. Am. Chem. Soc.* **2019,** *141*, 1435-1440.

3. Yen-Pon, E.; Buttard, F.; Frédéric, L.; Thuéry, P.; Taran, F.; Pieters, G.; Champagne, P. A.; Audisio, D. *JACS Au* **2021,** *1*, 807-818.

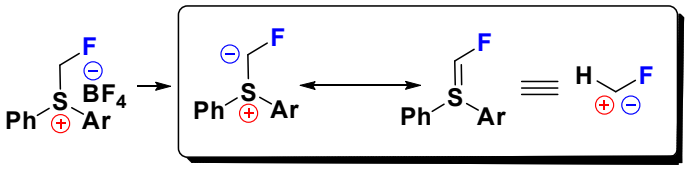
SULFONIUM REAGENTS FOR FLUOROMETHYLENE TRANSFER CHEMISTRY

Janis Veliks*

[a] *Latvian Institute of Organic Synthesis, Aizkraukles 21, LV-1006 Riga, Latvia*

** e-mail: janis.veliks@osi.lv*

Strategies to obtain monofluorinated organic compounds can be classified into two major categories: (1) synthetic routes that involve a direct fluorination step (formation of C–F bonds) and (2) the utilization of fluorinated building blocks. Both of these approaches are commonly used to access high-value fluorine-containing products. Fluoromethylene synthon can be considered as the smallest organic building block in fluorine chemistry. Our recent work demonstrates that monofluoromethylsulfonium reagents are solid, bench stable synthetic equivalents of the fluoromethylene synthon.[1-5]



1. J. Veliks, A. Kazia, *Chem. Eur. J.* **2019**, *25*, 3786-3789..

2. A. Kazia, R. Melngaile, A. Mishnev, J. Veliks, *Org. Biomol. Chem.* **2020**, *18*, 1384-1388

3. R. Melngaile, A. Sperga, K. K. Baldridge, J. Veliks, *Org. Lett.* **2019**, *21*, 7174-7178.

4. A. Sperga, E. Melngaile, A. Kazia, S. Belyakov, J. Veliks, *J. Org. Chem.* **2021**, *86*, 3196-3212.

5. A. Sperga, A. Kazia, J. Veliks, *Org. Biomol. Chem.* **2021**, *19*, 2688-2691.

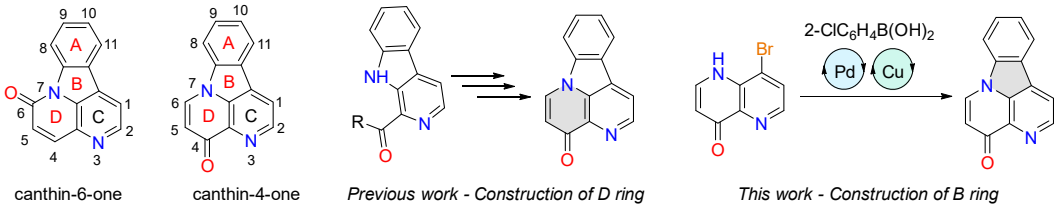
SYNTHESIS OF CANTHIN-4-ONE AND ISOCANTHIN-4-ONES VIA B-RING CONSTRUCTION

Maria Koyioni*, Panayiota Kelis and Panayiotis A. Koutentis

Department of Chemistry, University of Cyprus, Panepistimiou 1 Aglantzia, 2109, Nicosia, Cyprus

** e-mail: mkogio01@ucy.ac.cy*

Canthinones are a subgroup of *β*-carboline alkaloids, represented by canthin-6-ones[1] and canthin-4-ones. More than 40 natural analogues of canthin-6-ones have been isolated to date, but only three natural canthin-4-ones: tuboflavine,[2] norisotuboflavine,[3] and isotuboflavine[2] have been reported. While scarce, both natural and synthetic canthin-4-ones, have potential in medicinal chemistry as they exhibit antimicrobial activities, and phosphodiesterase-inhibitory activity.[4] Accessing diverse libraries of canthin-4-ones for structure activity relationship studies remains limited owing to the lack of good general syntheses. Early and recent routes to canthin-4-ones, are based on *β*-carboline precursors, proceeding *via* construction of the D-ring, thus diversification of the carboline backbone is limited.[5] Herein, we describe a short synthesis of canthin-4-ones, and isocathin-4-ones, *via* construction of the B-ring which enables, facile diversification of the A ring.



1. J. Dai, N. Li, J. Wang, U. Schneider. *Molecules*, **2016**, *21*, 493.

2. C. Kump, J. S. H. Schmid. *Helv. Chim. Acta*, **1963**, *46*, 498-505.

3. H. Achenbach, K. Biemann. *J. Am. Chem. Soc.*, **1965**, *87*, 4177-4181.

4. a) A. Puzik, F. Bracher. *J. Heterocycl. Chem.*, **2009**, *46*, 770. (b) T. Tremmel, A. Puzik, A. P. Gehring, F. Bracher. *Arch. Pharm. Chem. Life Sci.* **2016**, *349*, 710-723. (c) M. Ohashi, H. Nishida, T. Shudo: Compounds having CGMP-PDE inhibitory effect. US Patent 6,476,021 B1, 2002.

5. T. Tremmel, F. Bracher. *Tetrahedron*, **2015**, *71*, 4640-4646.

CATALYTIC FUNCTIONALIZATION OF C(SP^3)–H BONDS

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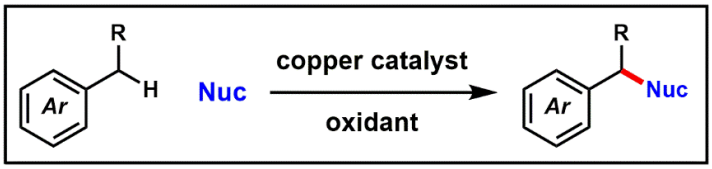
** e-mail: sokr@kemi.dtu.dk,*

Homepage: www.sorenkramer.com



Catalytic C–H functionalization offers an opportunity to access novel retrosynthetic disconnections and potentially shorten synthesis routes.[1] This presentation will cover our research efforts focused on development of new methods for catalytic functionalization of C(sp^3)–H bonds using metal catalysis. The primary focus of the presentation will be the development of new methods for copper-catalyzed benzylic C–H functionalization reactions, predominantly using imines as nucleophiles. Specifically, a copper-catalyzed route to α-substituted, primary benzylamines by C−H functionalization of alkylarenes is presented.[2] The method directly affords the amine hydrochloride salts. Catalyst loadings down to 0.1 mol% in combination with scalability, insensitivity to air and moisture, and no need for column chromatography makes the procedure highly practical. Preliminary mechanistic data is also discussed. Finally, our efforts toward the use of other nucleophiles as well as other types of C(sp^3)–H functionalization will be presented.[3,4]

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1. J. F. Hartwig, *J. Am. Chem. Soc.* **2016**, *138*, 2–24.

2. S. Kramer. *Org. Lett.* **2019**, *21*, 65–69.

3. M. B. Buendia, J.-G. J. Balin, M. E. Andersen, Z. Lian, S. Kramer. *Synlett* **2021**, doi: 10.1055/s-0040-1720474.

4. Unpublished results.

EFFICIENT SYNTHESIS OF LINEAR TRISACCHARIDE FROM QS-21

Đani Škalamera*[,a], Ivana Tuković[a]

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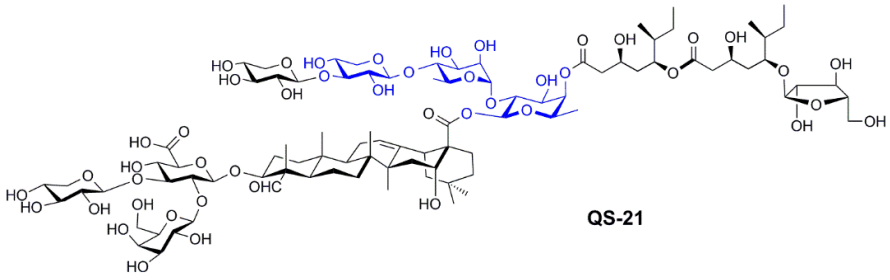
* *e-mail: dskalamera@chem.pmf.hr*

Adjuvants are key components of vaccines that improve and/or modulate the immune response to the applied antigen. The natural compound QS-21, a saponin isolated from the bark of *Quillaja saponaria* Molina tree, is one of the strongest known immunoadjuvants. However, QS-21 has a few major drawbacks which inhibit its wider use, e.g. chemical instability, accessibility and difficult purification; which led to the development of QS-21 derivatives and simpler variants. The linear trisaccharide Xyl(β1-4)Rha(α1-2)Fuc was found to be a crucial structural domain for the immunostimulatory activity of the QS-21 derivatives.[1] Thus, its efficient synthesis is very important in the further development of QS-21 derivatives and analogs. Currently reported syntheses of the trisaccharide have shortcomings in extremely moisture-sensitive glycosylations, relatively high number of steps and low total yields.[2]

In this work, a simple, efficient and robust method of glycosylation using glycosyl fluorides as donors and silyl ethers as acceptors was used for the synthesis of trisaccharide Xyl(β1-4)Rha(α1-2)Fuc. That led to the simplification of the synthetic pathway and reduction of the total number of steps, making the trisaccharide more easily accessible.



QS-21

1. A. Fernández-Tejada, D. S. Tan, D. Y. Gin, *Acc. Chem. Res.*, **2016**, *49*, 1741−1756.

2. (a) Đ. Škalamera, H. Kim, P. Zhang, S. M. Michalek, P. Wang, *J. Org. Chem.*, **2020**, *85*, 15837-15848; (b) E. K. Chea, A. Fernández-Tejada, P. Damani, M. M. Adams, J. R. Gardner, P. O. Livingston, G. Ragupathi, D. Y. Gin, *J. Am. Chem. Soc.*, **2012**, *134*, 13448−13457.

HOW MODERN CHEMISTRY CAN CONTRIBUTE TO SUSTAINABILITY OBJECTIVES.

André P. Dieskau*,[a]

[a] *Bayer Pharmaceuticals, Research & Development, Chemical Development, 42096 Wuppertal, Germany*

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In accordance with Paris Climate Agreement, Bayer AG – a Life Science Company – stands up to fight climate change and limit global warming to 1.5 °C.[1] We believe sustainability is not only a corporate responsibility but a business opportunity to drive growth. In Bayer Pharmaceutical's Chemical Development organization, we drive the development of new drugs to serve patients by innovative chemistry in line with the Green Chemistry principles. In this talk, we will present recent examples from our innovation pipeline and demonstrate *how modern chemistry can contribute to sustainability objectives.*

1. Bayer AG, Geschäftsbericht 2020

HOMOGENEOUS CATALYSIS IN ORGANIC TRANSFORMATIONS – A VIEW FROM INDUSTRY

Lucas Carreras*[,a]

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** e-mail: lucas.carreras@matthey.com*

The homogeneous transfer hydrogenation of ketones and imines[1] and catalytic hydrogenation of esters,[2] thanks to the recent advances driven by industrial and academic research groups, are established tools for industrial applications such as pharmaceutical, agrochemical or flavour & fragrances chemistry.

Key considerations for these catalytic processes such as cost and optimisation, as well as examples of industrial applications will be reviewed in the presentation.

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1. H. G. Nedden, A. Zanotti-Gerosa, M. Wills. *Chem. Rec.*, **2016**, *16*, 2623–2643.

2. A. Zanotti-Gerosa, D. Grainger, L. Todd, G. Grasa, L. Milner, E. Boddie, L. Browne, I. Egerton, L. Wong. *Chim. Oggi*, **2019**, *37*, 8–11.

REDUCING SYNTHETIC COMPLEXITY OF THE BACTOBOLIN CLASS OF RIBOSOME INHIBITORS

Jakub Švenda

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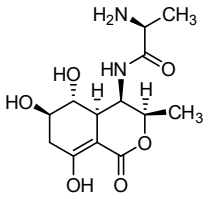
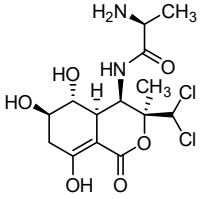
Bactobolins are complex natural products with broad spectrum antibacterial activity.[1] Biochemical and crystallographic studies have revealed that bactobolins inhibit protein synthesis and target a novel binding site within the bacterial ribosome that is not shared with any currently approved antibiotics.[2] Biomedical potential of these ribosome inhibitors is complicated by their toxicity toward eukaryotic cells, triggering a search for analogs with improved properties. My research group set out to reduce the synthetic complexity of bactobolins, seeking practical access to the fully synthetic analogs thereof. In this lecture, I will illustrate how strategic planning translated into efficient laboratory syntheses of (+)-actinobolin (**1**) and (–)-bactobolin A (**2**).[3]



(+)-Actinobolin (**1**)



(–)-Bactobolin A (**2**)

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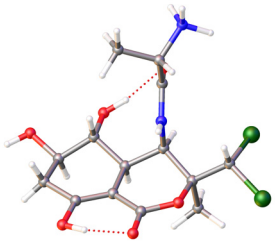

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DEVELOPMENT OF NOVEL CONTINUOUS-FLOW SYNTHESIS TECHNOLOGIES AND UTILIZATION THEREOF IN PEPTIDE AND FOLDAMER CHEMISTRY

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The importance of synthesis of peptides is warranted by the need for peptide-based medicines. Nowadays, peptide synthesis is performed almost exclusively on solid supports. The solid-phase peptide synthesis (SPPS) technique has subsequently been progressively developed. However, still a general drawback of these methodologies is the high number of amino acid equivalents required for total coupling.[1]

Continuous-flow (CF) technologies are of considerable current interest, since more efficient and selective reaction can be carried out in continuous systems than those for regular batch operations. These properties were utilized for the synthesis of peptides and foldamers under CF conditions with prominently low amino acid excess (1.5 fold of excess) and solvent consumption providing an exceptionally green technology.[2, 3]

The technology was further used for the sustainable construction of various amide bond containing compounds and for the synthesis of several deuterated aromatic molecules.[4]

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BIOCATALYTIC APPROACHES TO COMPLEX TARGETS

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The extraordinary selectivity associated with enzymes makes them extremely attractive catalysts for the synthesis of complex chiral molecules. The ability of these catalysts to operate under similar reaction conditions also means that it is possible to design multi-enzyme cascade reactions, were the product of one biocatalytic step becomes the substrate for the next enzymatic transformation. Such tandem systems can significantly reduce the number of synthetic manipulations and avoid costly purification steps, and as such, the design of such processes have become extremely attractive to industry. We are interested in the design of biocatalysts and biocatalytic methodology that can simplify synthetic routes to high-value targets. This talk will focus on some of our latest biocatalytic methodology developments and explore how they can help simplify synthetic approaches to challenging compounds.

MOVING FROM DIRECT PHOTOCHEMISTRY TO PHOTOREDOX CATALYSIS - A MECHANISTIC ADVENTURE

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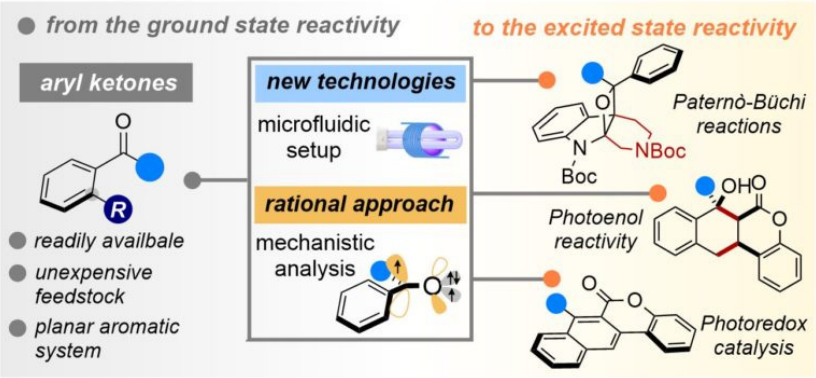
The technological advancements and the detailed mechanistic understanding of photochemical processes can unlock previously inaccessible reactivities.



We have exploited microfluidic photoreactors to enhance the synthetic performance and scalability of several photochemical methods including the phenol alkylation[1] and the trifluoromethoxylation of ketones.[2] Further, the careful mechanistic analysis of the developed methods has been instrumental to disclosing a new family of powerful organic photocatalyst able to mediate several thermodynamically extreme photoredox processes.[3]

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PHOTOCATALYTIC MODIFICATIONS OF ORGANIC HALIDES IN SELF-ASSEMBLED AQUEOUS SYSTEMS

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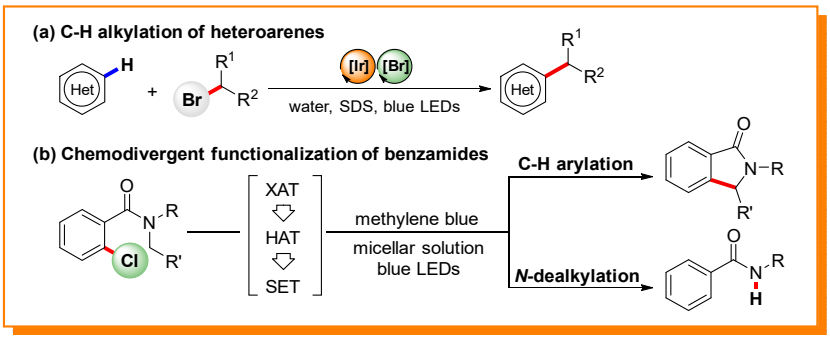
Organic halides, as readily available and inexpensive compounds, are desirable starting materials in photoredox catalysis.[1] Upon the mesolytic cleavage of the C–X bond, they form carbon radicals that can participate in further chemical transformations. While the synthetic potential of organic iodides has already been widely exploited, the photocatalytic activation of bromides and chlorides remains a current challenge.



Herein, we show the key role of non-covalent interactions in C-H alkylation of heteroarenes with alkyl bromides, and the functionalization of chlorinated benzamide derivatives.[2,3] Thanks to the use confined micellar media, it is possible to carry out the reaction under mild conditions, without the need for stoichiometric amounts of chemical reducing agents or radical promoters.

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STEREOSELECTIVE SYNTHESIS OF UNNATURAL α-AMINO ACIDS THROUGH PHOTOREDOX CATALYSIS

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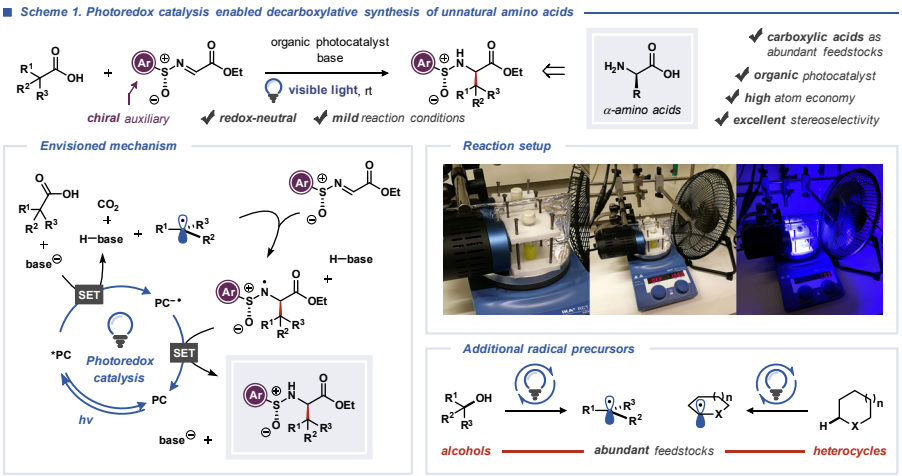
Chiral amine moieties are present in a variety of biologically active targets, such as amino acids, and heterocyclic motifs. An appealing approach for accessing amines involves C–C bond formation through alkylation of imines. Traditional two-electron manifolds revolve around nucleophilic addition to the C=N bond employing preformed organometallic reagents. However, these carbanion-type reagents display limited compatibility with electrophilic or acidic functional groups. The limitations associated with traditional organometallic reagents can be conquered with free radical-based methods.[1] Recently, our group became interested in the possibility of employing carboxylic acids to affect net redox-neutral, stereocontrolled alkylation of imines (Scheme 1).[2] Preliminary studies have demonstrated that other classes of compounds can also be employed as radical precursors. This work highlights the versatility of photoredox catalysis for engaging sp^3 carbon-centered radicals in radical manifolds with imines.



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SOLAR ENERGY DRIVEN SUSTAINABLE SYNTHESIS OF PHARMACEUTICALS AND FUELS

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Currently, human beings are completely dependent on the extended use of fossil fuels as primary energy resource. In contrary, solar energy, contains huge amount of energy.[1] The average intensity of the total solar irradiance is about 1366.1 Wm^{-2} which provides roughly 4.3x1020 J energy only in 1 h. Therefore, if it is harvested properly and is utilized in organic synthesis or in fuel generation, can provide sustainable solutions in the society.[2] In fact, a very small fraction of solar energy, about 0.1%, is converted by natural photosynthesis into biomass. Chemists are learning to exploit the huge amount of solar energy by artificial photochemical reactions for two important applications: (i) to convert sunlight into chemical or electrical energy, and (ii) to perform organic synthesis that cannot be obtained by conventional chemistry.[3,4] Light excitation of a molecule or a semiconductor leads to an electronically excited state capable of performing as a stronger one-electron oxidant/reductant compared to the ground state. This means that light excitation promotes a primary electron-transfer reaction. The primary photoinduced electron-transfer reactions can later be converted into desired products via radical formations during photocatalysis. Based on this consideration, we are working on the synthesis of pharmaceuticals, fine chemicals and fuel type molecule generation.

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HARNESSING PHOTOCHEMISTRY IN RADIOTRACER SYNTHESIS

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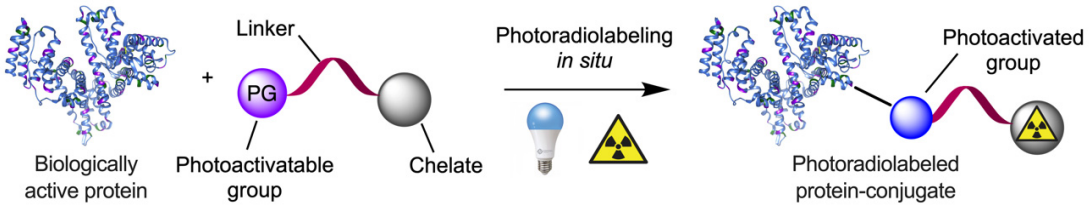
Photochemistry harbours many fascinating reactions and reactive intermediates that hold potential for applications in the synthesis of bioactive compounds. In recent years, my group has been exploring the use of compounds that undergo light-induced activation for the synthesis of protein-conjugates like monoclonal antibodies functionalized with radioactive metal complexes, fluorophores, and drugs. Photolysis typically produces extremely reactive, short-lived intermediates (with lifetimes in the micro-to-picosecond range) and controlling the experimental conditions to allow productive bioconjugation chemistry is the major challenge in harnessing light-induced chemistry. This presentation will introduce some of our recent synthetic, spectroscopic, computational, radiochemical, and biological studies using (automated) photoradiosynthesis to make viable radiotracers in a flash.[1-5]



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FLUORINATED POROUS ORGANIC CAGE COMPOUNDS

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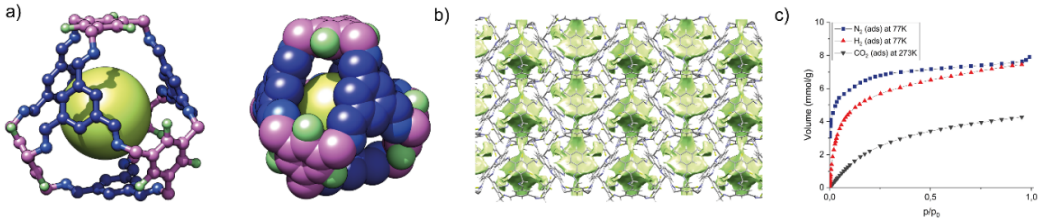
Supramolecular chemistry has continued to evolve in recent decades and has successfully found its way into nanotechnology and materials. In addition to the properties of metal-organic frameworks (MOFs) and metal-organic cages, covalent-organic frameworks (COFs) and porous dynamic-covalent cage compounds (POCs) have attracted tremendous attention in the past years.[1,2] We focus on the synthesis and characterization of novel POCs by inverting the electron density of the aromatic panels used for the self-assembly by fluorination. These cages show distinct gas adsorption properties and significantly increased thermal stabilities, exemplarily shown by the synthesis of the first highly fluorinated, porous, organic Tri^{4}Tri^4 imine cage, **FC1**, containing perfluorinated aromatic panels and hydrogenated panels.[3]



Gas adsorption experiments show an uptake of 19.0 wt% CO_2 (4.2 mmol g^{-1}, 273 K and at 1 bar) and 1.5 wt% H_2 (7.5 mmol g^{-1}, 77 K and at 1 bar) for the specific surface area of 536 m^2 g^{-1} of the crystalline **FC1** material obtained directly from the reaction mixture.[3] Additionally, the unique reactivity of the employed building blocks will be showcased by studies regarding organic Tri^{4}Di^6 imine cages,[4] and Di^{3}Di^3-type macrocycle formation.[5]

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INTEGRATING THE HAMMETT EQUATION INTO COVALENT ADAPTABLE IMINE NETWORKS

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Traditionally, polymers can be either classified as thermoplastics (*i.e.*, easily processable polymer with limited mechanical strength), or as thermosets (*i.e.*, (networked) polymers that are mechanically strong but lack the ability to be straightforwardly processed or recycled). While the permanent network structure in the latter class of polymers imparts these materials with mechanical robustness, the same permanent network precludes simple (thermal) processing. Only in this last decade, a solution to these seemingly irreconcilable objectives of robustness and processability, was put forward: covalent adaptable networks.[1] In these networks, individual polymer chains are connected via dynamic-covalent bonds, which allows rearrangement of the network. This results in polymer materials that combine mechanical strength with more facile (re)processing.

To fully deliver on the great promise of dynamic-covalent chemistry –and of the derived covalent adaptable networks– for the development of robust polymers that are recyclable, reprocessable or self-healing, new design strategies towards these materials are needed. In this contribution, the well-established physical-organic concept of the Hammett equation, operative at the molecular level, will be presented as a fine-tuned design strategy to control dynamic material properties on the macroscopic level.[2] Focusing on polyimines, the possibility to tune their dynamic mechanical and thermal properties via the electronic effect of dianiline monomers based on the Hammett equation will be presented. The dynamic nature of the imine bond will also be shown to enable recycling and intrinsic self-healing of the materials over multiple cycles without any external input.

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FT-IR SPECTROSCOPY AS A SIMPLE TOOL FOR RAPID SOLUTION OF VARIOUS PROBLEMS

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FTIR spectroscopy is non-destructive and simple analytical technique that requires small sample amounts for providing information about functional groups in molecules. In certain cases, it is indispensable for structure elucidation of complex organic molecules such as triterpene derivatives[1]. Applying this technique, it is possible to monitor the change in the secondary structure of the protein.[2].

Combined with various statistical methods it is a powerful analytical tool in metabolomics. Thus, FTIR data based statistical models enabled propolis classification and floral origin determination[3]. In combination with biological tests such as cytotoxic activity), it can be used for biologically guided isolation of active compounds[4].

Nowadays FTIR spectroscopy is being routinely used for solving various practical analytical problems, e. g. quality analysis of bees products (beeswax and honey), quantitative determination of the major constituents in most types of food and agricultural products, straightforward identification of kidney and bladder stones etc.

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DATA-DRIVEN MODELING OF BIOORTHOGONAL REACTIONS

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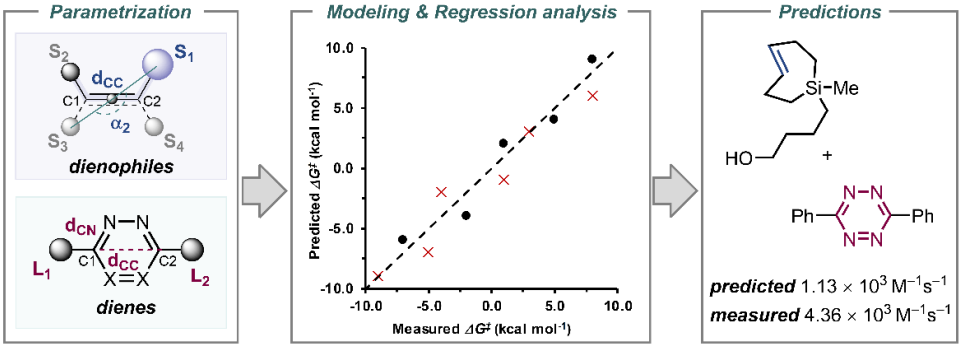
Bioorthogonal reactions, such as cycloadditions, are widely used for probing and controlling biological functions through labelling, tracking and imaging of biomolecules. Advances in the bioorthogonal toolbox have rendered these reactions more effective, selective and widespread, which continues enabling the construction of innovative theragnostic and delivery systems for in vivo applications.[1]

Fundamental determination of reaction kinetics is commonly performed by transition state analysis using density functional theory (DFT) calculations.[2] Herein we show a complementary, modern data-analysis approach[3] by parametrizing the cycloaddition reagents and solvents (Figure 1).[4] In this approach we use chemically comprehensible and easy to calculate descriptors to developed models that are statistically robust and have good predictive skills.



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TURNING SIMPLE HYDROCARBONS INTO MULTIFUNCTIONAL BUILDING BLOCKS

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The development of efficient, safe, clean and operationally simple transformations is a primary challenge in modern synthetic chemistry. Traditionally, transition metal catalyzed C-C bond forming reactions have been developed using pre-made organometallic reagents. These procedures are inherently limited to the availability and reactivity profiles of the reagent itself and entail the formation of a stoichiometric amount of inorganic salt as a reaction by-product. The goal of our research program is to discover and study new metal-catalyzed reactions with the aim to develop highly selective synthetic methodologies based on the use of readily accessible materials. In this context, we have recently developed new synthetic transformations based on the use of simple unsaturated hydrocarbons as transient functionalized organometallic intermediates in multicomponent reactions.[1-4] From simple and readily available materials we can obtain complex structures with a high level of selectivity.

In this lecture, different catalytic strategies to accomplish difunctionalization of unsaturated hydrocarbons based on selective carboboration processes will be presented.

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A MULTICOMPONENT TETRAZOLO INDOLE SYNTHESIS

Constantinos G. Neochoritis*[,a], Xiaofang Lei[a,b], Panagiota Lampiri[a], Pravin Patil[b], Giasemi Angeli[a] and Alexander Dömling[b]

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[b] *University of Groningen, Department of Pharmacy, Groningen, The Netherlands.*

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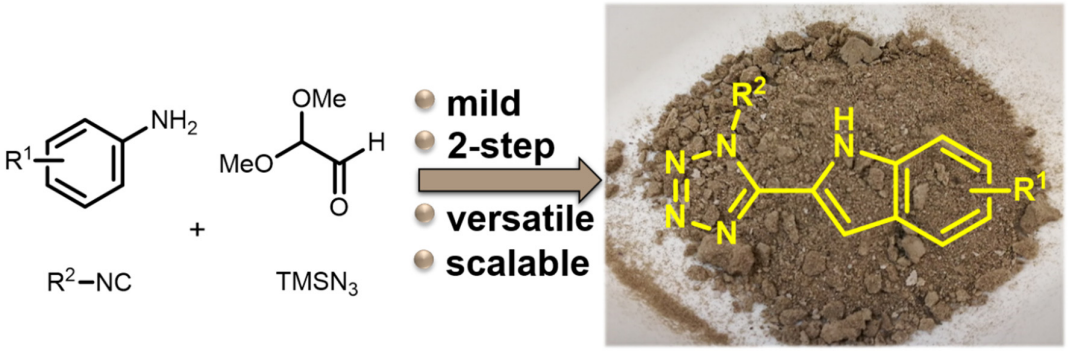
The ubiquitous presence of the indole fragment in natural products and drugs asks for ever novel syntheses. We report an unprecedented mild, two-step synthesis of 2-tetrazolo substituted indoles based on the Ugi-tetrazole reaction combined with an acidic ring closure. A gram-scale synthesis, a bioactive compound and further transformations were performed.



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α-*gem*-DIBORYL CARBON-CENTERED RADICALS: TOWARDS SYNTHETIC DIVERSITY

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Our main goal is to explore the reactivity of a currently not studied reactive species, namely, the α-*gem*-diboryl carbon-centered radicals (**II**).[1] The existence of these species was proposed in 2000 by Walton's research group.[2] However, until recently, these species have been considered as elusive.[3] In 2020, our group reported their synthesis and structural characterization.[4] We also demonstrated that these radicals are useful synthons and can be utilized for late-stage modifications of natural compounds. Thus, this chemistry aims at further exploration of the nature of these new and fascinating reactive intermediates that represent a complementary reactivity to *gem*diboryl-stabilized carbon-centered anions (**I**), which are currently well established and highly used in synthetic and material chemistry (Figure 1).[5]

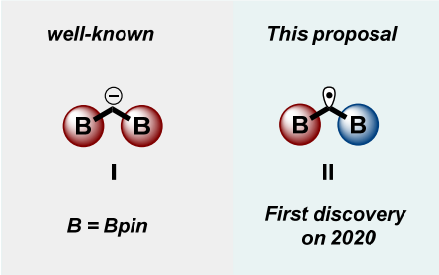

Figure 1.

We strongly believe that providing fundamental knowledge to the synthetic community will contribute much to better understand their reactivity and functionalization. We also believe that these new reactive intermediates (**II**) have the potential to be utilized for multiple stereoselective functionalizations of natural products, and even for bioactive molecules.

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STEREOSELECTIVE SYNTHESIS OF SPECIALIZED PRO-RESOLVING LIPID MEDIATORS

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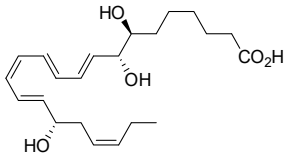
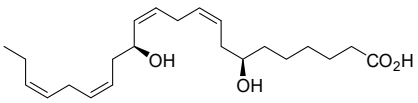
Specialized pro-resolving lipid mediators (SPMs) are polyunsaturated hydroxylated fatty acids with anti-inflammatory properties and pro-resolving actions. The SPMs play an active part during the resolution of inflammation.[1] These autacoid natural products protect organs, stimulate resolution, induce tissue regeneration as well as displaying significant effects against several human ailments, often in the nanomolar range.[1] Hence, they are potential leads towards drug discovery.

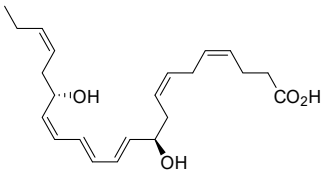
A summary of several total syntheses of various SPMs will be presented. LC-MS/MS results of the synthetic materials have been matched with endogenously produced SPMs allowing assignment of the absolute configuration of these lipid mediators.[2]



RvD1$_{n\text{-}3\ DPA}$



MaR1$_{n\text{-}3\ DPA}$



PD1

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CATALYTIC DIFUNCTIONALIZATION OF ALKENES WITH CHIRAL TRANSIENT DIRECTING GROUPS

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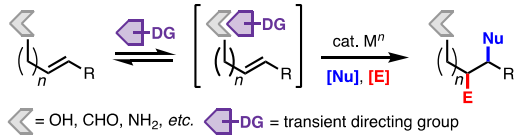
Catalytic alkene difunctionalization is powerful means of converting widely available starting materials into structurally complex products that would otherwise be problematic to synthesize. During the past few years, our lab and others have employed substrate directivity as a strategy for enhancing reactivity, controlling regioselectivity, and suppressing off-cycle pathways in catalytic alkene functionalization.[1,2] Many of these methods rely on removable bi/tridentate auxiliaries that must be installed and cleaved, requiring at least two concession steps and introducing inefficiencies into the synthetic workflow.[3–5] This seminar will describe the development of an alternative strategy that employs a (co-catalytic) transient directing group (TDG) to reversibly coordinate the substrate and recruit the metal catalyst of interest (Eq. 1).[6,7] We will examine the genesis of this idea, successful cases studies, and roadblocks faced along the way.

(1)



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SUSTAINABLE SYNTHESIS OF PHARMACEUTICAL INTERMEDIATES USING ELECTROCHEMICAL METHODS

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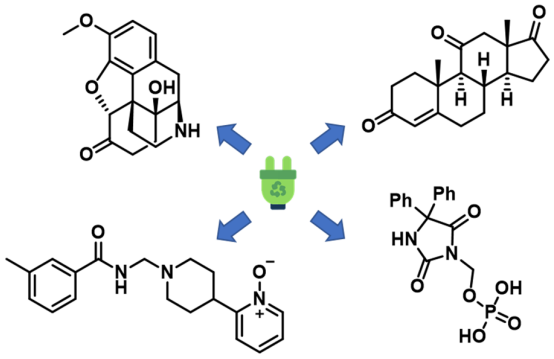
Electroorganic synthesis has seen a significant resurgence in recent years as an inherently sustainable methodology to effect redox processes.[1] Electrochemical methods have the capacity to generate radicals and other high energy intermediates under mild conditions, substituting stoichiometric amounts of often harmful and environmentally unfriendly oxidizing or reducing agents by electrical current.

Herein, we present selected examples from our group of challenging synthetic steps toward pharmaceutical ingredients of industrial relevance in which electroorganic synthesis has been applied as a green enabling technology.[2]



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AMPING UP ORGANIC SYNTHESIS WITH ELECTROCHEMISTRY

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Owing to its many distinct characteristics, electrochemistry represents an attractive approach to discovering new reactions and meeting the prevailing trends in organic synthesis. In particular, electrocatalysis—a process that integrates electrochemistry and small-molecule catalysis—has the potential to substantially improve the scope of synthetic electrochemistry and provide a wide range of useful transformations. In the past few years, we developed a new catalytic approach that combines electrochemistry and redox-metal catalysis for the functionalization of alkenes.[1] This talk details our design principle underpinning the development of electrocatalytic alkene difunctionalization and hydrofunctionalization with a particular emphasis on enantioselective electrocatalysis.[2] In addition, our recent forays into electrophotocatalysis will be discussed, in which we harness the power of both electricity and light to access catalytic species with exceptionally high oxidizing or reducing potentials.[3] Finally, the application of deep reduction electrochemistry in the context of alkene functionalization and cross coupling reactions will be discussed, wherein the combination of electrochemistry and physical organic chemistry principles leads to previous challenging organic transformations.[4]

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NEW METHODS IN HALOGEN-ATOM TRANSFER (XAT)

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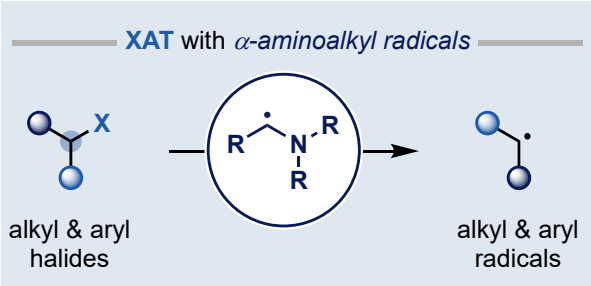
Organic halides are valuable building blocks for the generation of alkyl and aryl radicals. However, their applications in photoredox catalysis can be difficult owing to their very negative reduction potentials.

We have recently demonstrated that strongly reducing systems are not required for the homolytic activation of these species under photoredox conditions. This is due to the unique ability of α-aminoalkyl radicals to undergo halogen-atom transfer with alkyl/aryl iodides and alkyl bromides.[1]

This blueprint for halide activation has been applied to the development of Giese reactions, radical allylation processes as well as Heck-type cross-couplings with styrene acceptors. Furthermore, integration of XAT reactivity with copper catalysis has been used for the SN2-like alkylation of secondary alkyl iodides with many N-nucleophiles.[2]



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