

ISy Sy Cat

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International Symposium on Synthesis and Catalysis

ÉVORA
September 5 - 8

Book of Abstracts



UNIVERSIDADE
DE ÉVORA



SOCIEDADE PORTUGUESA DE QUÍMICA

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Welcome

On behalf of the Organizing Committee I am very pleased to welcome you to the fifth edition of the International Symposium on Synthesis and Catalysis (ISySyCat2023) once again at the historic University of Évora. The inaugural edition of this conference that took place in September 2015 (ISySyCat2015) was a great success and from that moment we have been building on this success, making this a regular biannual event, which we can be proud of, and can put our country on the map. The conference focuses on various aspects of organic, organometallic and inorganic synthesis, as well as all areas of catalysis, including metal-based catalysis, organocatalysis and biocatalysis as well as polymer, soft material and inorganic synthesis. Issues of current major interest will be discussed, which include the sustainable production of important bulk, high-added value, continuous flow chemistry, photo-redox processes, electrosynthesis, enantiomerically pure compounds and biologically active compounds, from both academic and industrial perspectives.

To vindicate the resilience of this conference, ISySyCat21 successfully took place in September 2021, despite the COVID-19 pandemic. It was successfully organized as a hybrid conference, with both in person and on-line speakers and participants. It was a very memorable and rewarding event for us.

We are proud to have a delightful mixture of both academic and industrial chemists from all corners of the globe, making this yet again a very international event. This is also reflected in the fine line-up of speakers, which includes well-known experts and up-and-coming “rising” stars. There is also a very extensive line-up of oral and short oral presentations who in the main are junior researchers, post-docs or PhD students with some tantalizing research to discuss. Besides, there will be a smorgasbord of poster presentations, covering all aspects of these pivotal areas. Prizes will be awarded (to be announced during the Gala Dinner) for the best oral and poster presentations.

This conference should be the ideal venue for updating you on current developments and advances in these areas, for net-working, making new acquaintances, and at the same time allowing you to relax, soak up and enjoy the special surroundings, along with the unique food, drink and hospitality provided by this special region of Portugal.

We are very grateful to the Portuguese Chemical Society (Sociedade Portuguesa de Química), the University of Évora, and all our generous sponsors and supporters, without their valuable support this special event would not be possible.

We thank Wiley, Thieme and the RSC for making available prizes for the best oral and poster presentations.

We also thank Beilstein Organic Chemistry for running a special edition of this conference.

Last, but not least, we would like to thank all the participants at ISySyCat2023 for attending this conference and travelling from various parts of the world.

We hope that your participation will be rewarding, fulfilling, and of course, very pleasurable.

So, make the most of it and enjoy!

Anthony J. Burke
(Conference Chair)

Organization

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Narcisso Garrido, University of Salamanca, Spain

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SPQ office staff member: Cristina Campos

Abstract Book Editors

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Acknowledgments and Sponsors

The Organizing Committee is very grateful to the following companies and organizations for their kind sponsorship and support of ISySyCat_2023.

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Prize Sponsors



Wiley-VCH has very kindly agreed to sponsor a prize for the best oral communication. The winner will be announced during the gala dinner on the night of the 7th of September at the Hotel M'AR De AR Muralhas.

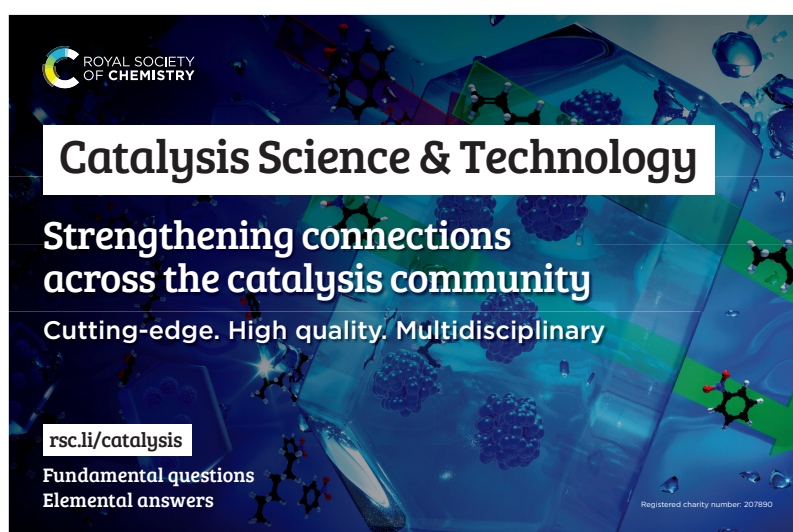
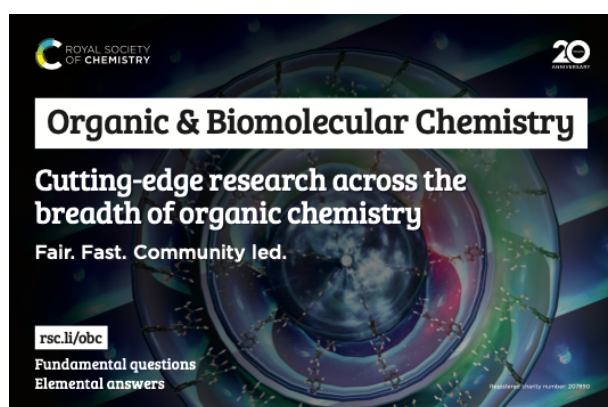


Thieme has very kindly agreed to sponsor two poster prizes. The winner will be announced during the gala dinner on the night of the 7th of September at the Hotel M'AR De AR Muralhas.



We are very grateful to the Royal Society of Chemistry (RSC) for sponsoring four best poster prizes, through their journals; Organic & Biomolecular Chemistry, Catalysis Science and Technology, RSC Sustainability and RSC Sustainability. Each winner will receive a prize worth of £100.





Media Partner



Chimica Oggi – Chemistry Today is a peer reviewed, bimonthly journal, of the TKS TeknoScienze Publisher. It deals with Fine Chemicals, Applied Chemistry and Biotechnology.

Founded in 1983 Chimica Oggi –

Chemistry Today soon became a leading journal in linking industry and academia and gained an immediate appreciation worldwide.

Open Chemistry is a peer-reviewed, open access journal that publishes original research, reviews, and communications in the fields of chemistry in an ongoing way. The central goal is to provide a hub for researchers working across all subjects to present their discoveries, and to be a forum for the discussion of the important issues in the field.



Advanced Synthesis & Catalysis (ASC) is the leading primary journal in organic, organometallic, and applied chemistry.

The high impact of ASC can be attributed to the unique focus of the journal, which publishes exciting new results from academic and industrial labs on efficient, practical, and environmentally friendly organic synthesis. While homogeneous, heterogeneous, organic, and enzyme catalysis are key technologies to achieve green synthesis,

significant contributions to the same goal by synthesis design, reaction techniques, flow chemistry, and continuous processing, multiphase catalysis, green solvents, catalyst immobilization, and recycling, separation science, and process development are also featured in ASC.

The **Beilstein Journal of Organic Chemistry** is an international, peer-reviewed, Open Access journal. It provides a unique platform for



**BEILSTEIN JOURNAL
OF ORGANIC CHEMISTRY**

rapid publication without any charges (free for author and reader) – diamond open access. The content is freely accessible 365 days a year to any user worldwide. Articles are available online immediately upon publication and are publicly archived in all major repositories. In addition, it provides a platform for publishing thematic issues (theme-based collections of articles) on topical issues in organic chemistry.

We are thrilled to announce that Beilstein Journal of Organic Chemistry will be running a thematic issue of ISySyCat23, which will be open to all contributors at ISySyCat23

INVITATION TO PUBLISH IN THE SPECIAL EDITION OF ISYSYCAT23 PUBLISHED BY BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

Dear Participant of ISySyCat 2023,

We cordially invite you to submit your most exciting, original research to be published in the Thematic Issue “5th International Symposium on Synthesis and Catalysis (ISySyCat 2023)” in the nonprofit, peer-reviewed *Beilstein Journal of Organic Chemistry* ([BJOC](#)).

This thematic issue is dedicated to the 5th International Symposium on Synthesis and Catalysis (ISySyCat 2023). Submission is open to all participants of the meeting and their co-authors.

The focus is on current themes of chemical synthesis and catalysis, for example, total synthesis and synthesis in medicinal chemistry, chemical biology, and materials science. Topics covered are new reagents, catalysts, strategies and concepts for organic synthesis, biocatalysis, organocatalysis, flow chemistry, process development towards the synthesis of key pharmaceutical targets, applications of organometallic compounds in synthesis and catalysis, stereoselective synthesis, synthesis and properties of functional molecules and organic materials, sustainable and green synthetic and catalytic methods, computational tools for synthesis and catalysis, and polymer synthesis.

Why choose *BJOC*?

The *Beilstein Journal of Organic Chemistry* is a true open access journal (no cost for authors and readers) and fully Plan S-compliant. We are funded entirely by the Beilstein-Institut, a charitable non-profit foundation that supports the communication of high-quality science without barriers. Benefits of publishing in *BJOC* include:

- Important specialist journal in the field of organic chemistry
- Diamond open access (no cost for authors or readers)
- Rapid publication
- Peer review to high standards (2–3 referees per paper)
- High production and online presentation standards
- Authors retain copyright and can reuse their work
- Article indexing and archiving
- Focus on quality, not profit

Thematic Issues

A thematic issue is a collection of articles dedicated to a focused topic. These issues are edited by guest editors who are experts in the respective field and aim to stand out as valuable and unique reference works.

How to Submit

The submission deadline for this thematic issue is **December 15, 2023**. We would greatly appreciate if you could let us know via email by **September 14th, 2023** (this date was extended from the 15th of August) whether you intend to submit a paper, and if so, in which format (review, research article, letter, or perspective). Please contact Dr. Marc Kielmann of the editorial office (mkielmann@beilstein-institut.de)

To submit your article, please upload it directly to the Beilstein Publishing System at <https://www.beilstein-journals.org/bps/> and ensure that the submitting author includes the following information in the cover letter:

Thematic Issue: 5th International Symposium on Synthesis and Catalysis
(ISySyCat 2023)

Corresponding Editor: Anthony J. Burke

Please find further information on the submission process at www.beilstein-journals.org/bjoc/submissionOverview and feel free to consult the *Beilstein Journal of Organic Chemistry* Editorial Team (bjoc-editorial-office@beilstein-institut.de) in case you have questions regarding the submission and processing of your article.

Given your expertise in the field, we would be very pleased to receive a manuscript submission from you, and we look forward to hearing from you on your acceptance to this invitation.

Best wishes,

Anthony J. Burke (Guest Editor) and Marc Kielmann (Managing Editor)

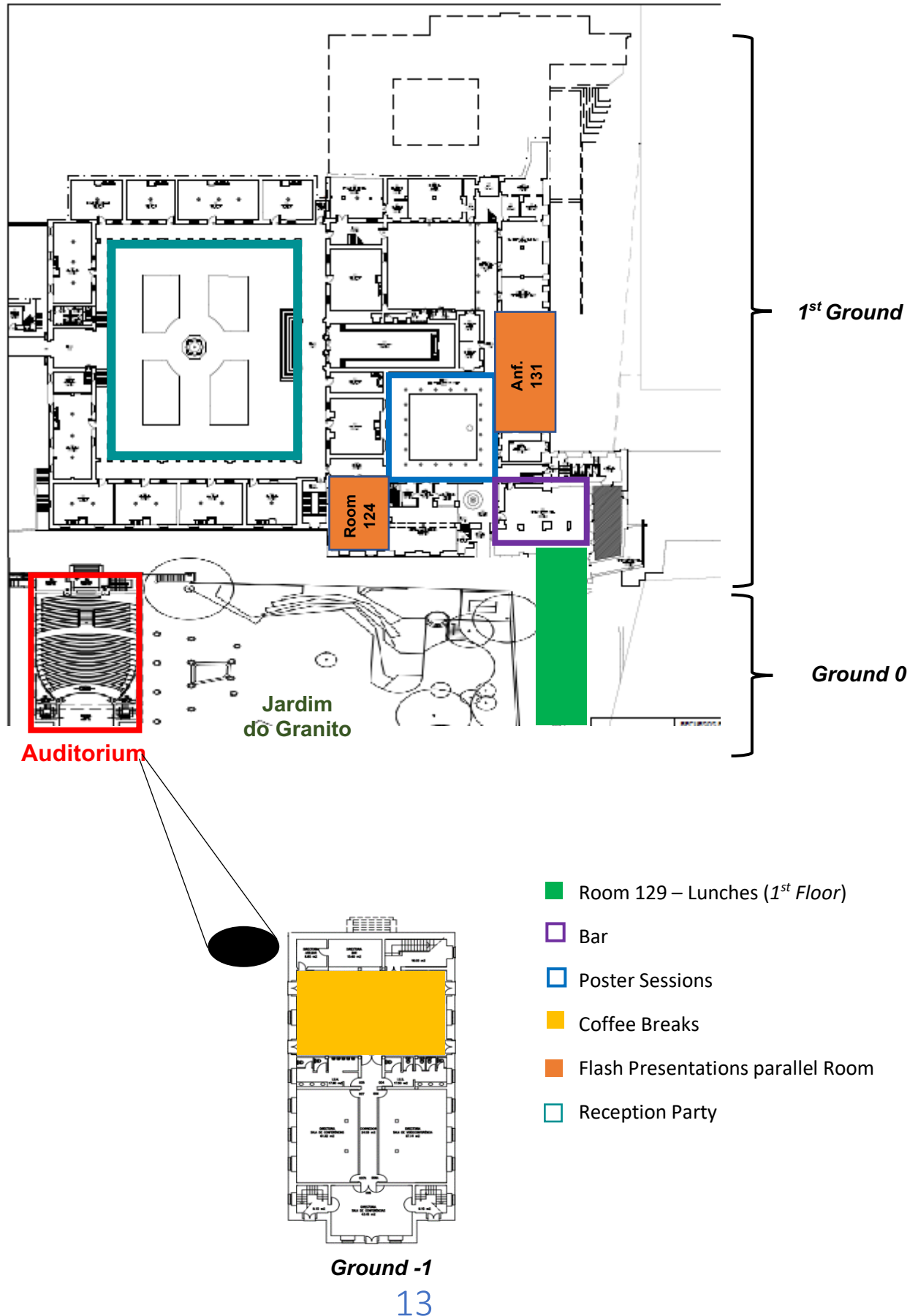
General Information

Meeting Venue

The meeting will take place at the auditory of Colégio Espírito Santo (CES) located in University of Évora, Largo dos Colegiais, number 2, 7004-516 Évora, Portugal.



Inside the CES building, the main conference room (the Auditorium), the speaker's preview rooms, poster session venue, exhibition and coffee break areas will be appropriately signposted, as illustrated in the map below.



Important and useful information

Access and stay at the Venue

Suitable identification (corresponding name badge) should be used by all the attendants, during the meeting.

Lunches

Lunches on Tuesday 5, Wednesday 6 and Thursday 7 of September will be served at the room 129 of CES and are included in the registration fee. We kindly ask all participants to use their ID badge to access lunch area.

Internet Access

A temporary login for the wireless Academic Network (eduroam) for the University of Évora has been created (valid from 30th of August to 11th of September). Please use the following credentials:

Username: isysycat2023

Password: Uevora9775

Scientific Information

Presentation Preview Room

To ensure that sessions run on time, speakers are kindly asked to provide the oral communication files in advance, preferably 24 h before their presentation. Please use the following email address to send your communication: isysycat2023.pres@gmail.com.

Oral presentations will be in PowerPoint on a Windows OS. Therefore, Mac users should verify that their presentations work well in a Windows environment. If you intend to use your computer, please inform us by e-mail (isysycat2023.pres@gmail.com) in advance.

Flash Sessions

On the 5th, 6th and 7th of September three parallel Flash session presentations will take place in the main Auditorium, in Room 131 and in Room 124. The talks will have a maximum time of 10 minutes each.

Poster Sessions

Posters will be displayed in the selected halls of CES. Authors are requested to display their posters on the post panels during the first coffee break (or lunchtime) on the 5th of September. Material to attach posters will be made available by the organizing committee at the front desks. Posters should be on display from Tuesday morning and left for the entire Conference (remove them by the coffee break on the last day (8th of September)). Authors are requested to stay near their posters during the assigned session so they will be available to answer any questions from the participants and by the evaluation panel, who will select the posters for the Poster Prize awards.

Awards and Prizes

In ISySyCat 2023, a number of exciting Awards will be given, for both the best Oral and Poster communications.

Oral Talks

Wiley-VCH Verlag GmbH & Co. KGaA – A company of John Wiley & Sons, Inc, has very kindly agreed to sponsor a textbook for the best oral communication.

Poster Prizes

Thieme Group Stuttgart have very kindly agreed to sponsor two poster prizes, consisting of a one-year subscription to SYNFACTS and the corresponding certificate.

Royal Society of Chemistry, through its affiliated journals (RSC Sustainability, Reaction Chemistry & Engineering, Organic & Biomolecular Chemistry and Catalysis Science & Technology) have very kindly agreed to sponsor four poster prizes, that includes a certificate and a cheque for £100.

Language

English is the official language of ISySyCat 2023.

Other information

Time Zone: The time zone in Portugal is GMT.

Water: Tap water in Portugal is drinking water.

Electricity: In Portugal, the line voltage is 220 V and the connection is made by a two-pin plug. Travelers from the USA will require a voltage converter. Travelers

from the UK will require a plug adapter, and this is best bought in the UK as they are hard to find in Lisbon (can try at the Lisbon airport).

Currency, Banks and Post Offices: The national currency in Portugal is Euro. Banks are open from Monday to Friday between 8.30 am and 3 pm. Post offices are usually open between 8.30 am and 6 pm. Exchange houses operate everyday between 9 am and 1 pm and from 2 pm to 7 pm.

Going out in Évora: With your conference material, you will find a city map and a brochure of Évora with lots of necessary information.

Climate: In early September, the temperature in Évora is on average 30°C (the nights are hot). Rain is very unlikely.



Social Programme

Reception Party *(included in the registration fee):*

The reception party will be in the CES cloisters on Tuesday the 5th of September at 19:40h. It will include appetizers, drinks and a live DJ.

Banquet Dinner *(included in the registration fee):*



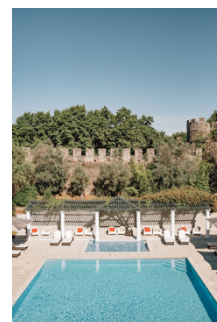
On Thursday the 7th of September at 20:00h, the conference Gala Dinner will take place at the Hotel M'AR De AR Muralhas, a 4-star hotel just within the main city walls. The buffet dinner will consist of a fine selection of local and regional dishes and wines, and other beverages, that will be preceded by a pleasant outdoor (garden) cocktail reception. We greatly look forward to sharing your company.

M'AR De AR Muralhas is a timeless charm Hotel in the historic center of the city of Évora, right in the heart of the area classified by UNESCO as World Heritage. Quality is here a synonym of a warm and friendly welcome.



Located on the ground floor, facing the garden and the swimming pool, the Restaurant *Sabores do Alentejo* has the signature of Chef António Nobre. Menu's privilege local innovative cuisine, based on regional flavors and delicious, surprising combinations. The atmosphere is cozy and comfortable. Natural light makes it very attractive for lunch, and the outside porch, facing the pool, is the ideal place for dinner in a warm summer night.

M'AR De AR Muralhas offers beautiful gardens, where you can enjoy the beauty of the historic surrounding city wall, relaxing on the porch or by the swimming pool while drinking a delicious cocktail.



Excursion on the 8th of September *(not included in the registration fee with limited seats):*

On the afternoon of the 8th of September, conference participants are invited to part-take in a delightful social program to the famous **Quinta da Plansel** (<https://www.plansel.com>) in Montemor-o-Novo (a typical Alentejo town, 30 km outside of Évora). After a welcoming cocktail, it will be served a beautiful three course set lunch, accompanied by a selection of excellent wines, including wine tasting from the Quinta da Plansel wine cellar, and a guided visit to the winery. As the visit will coincide with the peak of the active and busy vine harvesting season, it should be an interesting experience. Full details can be seen below and will be given during the conference.



Important Note: Persons with dietary restrictions should indicate this on the registration form (preferentially) or in the registration desk during the conference so that an alternative can be arranged.



Quinta da Plansel was born out of a misunderstanding by its founder, Jörg Böhm, when in 1961 his sailing boat sank in the port of Cascais. Forced to stay here for some time, he ended up getting to know and surrendering to different Portuguese landscapes. And that's how he saw the huge winegrowing potential of the Alentejo grape varieties, and in 1975 he bought the first land for vineyards and set up Viveiros Plansel.

This family has always been connected to wine. The first records date back to the 11th century, but from the 18th century onward the Böhm family's



mission to the industry became more evident, being one of Germany's leading wine importers and distributors. The passion for wine and for Portugal would eventually infect the whole family. In the early 1990s, daughter Dorina Lindemann, an oenologist with a degree from the University of Geisenheim (Hessen), came from Germany to Portugal with her husband Thomas Lindemann and, taking advantage of the existing vineyards linked to her father's technical improvement program, dedicated herself to wine production.



With the young engineer Paulo Laureano, Dorina Lindemann produced her first wine at the Adega Experimental da Mitra ([University of Évora](#)), in 1993. The first brand was Plansel (which means from Selected Plants). Over the next five years, Dorina and her husband, Thomas, built their own winery, Quinta da Plansel.

Dorina's goal was to transfer all of her father's basic knowledge to oenology. The revival of old varieties was the secret of the differentiation of these wines, both in quality and quantity. Currently, daughters

Júlia and Luísa are also part of the wine business, from marketing to oenology, ensuring the future of the project.

Today, the winery reaches an annual production of 400,000 liters, having diversified its products into five different ranges, with wines of very unique profiles. Quinta da Plansel is mainly known for its work with the Touriga Nacional, Touriga Franca, and Tinta Barroca grape varieties, its favorites.



The very specific microclimate of Montemor-o-Novo, with a maritime influence and sheltered from the hot southerly winds by the small mountains, turned out to be beneficial to the vines, making them more resistant to the drier year.

Despite the challenges, we believe that the references signed by the year 2022 will be very rich, both in the nose and in the mouth. Now we just have to wait a few years to taste them.



- Walking Guide tour to Évora (included in the registration fee):

The participants who are interested in this tour should contact the staff on the first day of the conference to book their place (limited to 100 participants). It will be on the 8th of September at 15h. The meeting point will be in the Tourist Office in Giraldo's square and will end in the bone chapel around 16:30h. The participants should present the corresponding badge of the conference.

Évora was considered a world heritage place by UNESCO in 1986. According to this organization, Évora is a museum-city with roots dating back to roman times. The golden age happened in the 16th century, when the Portuguese kings lived here. Among many others, the old wall, the aqueduct, medieval buildings like the cathedral, convents, palaces, churches and squares are convincing reasons for a walking tour. Some of the highlights in Évora are the architecture of the white houses, the tiles and the balconies. Come and see these places with your own eyes.



*The light that illuminates you,
Land the color of the eyes of those who look!*

Miguel Torga (Portuguese writer)



The tour itinerary is:

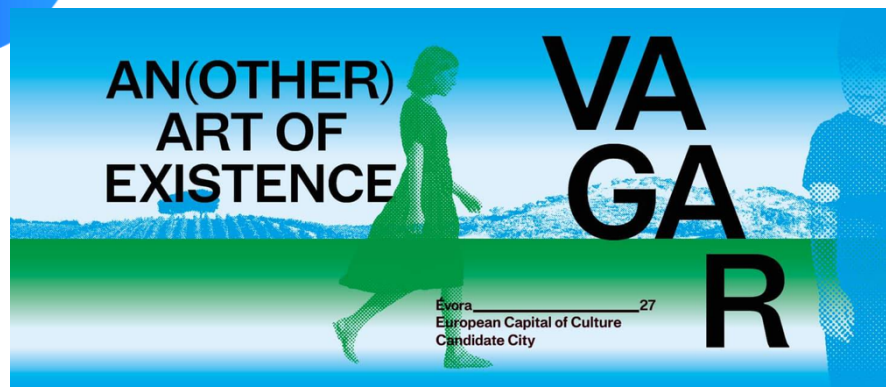
- ⇒ Praça de Giraldo (Giraldo's square)
- ⇒ Rua 5 de Outubro (5th October street)
- ⇒ Catedral (Cathedral, to visit inside a fee must be paid per person, or you can enjoy only outside)
- ⇒ Templo Romano (Roman Temple, Diana's Temple)
- ⇒ Jardim Diana (Diana's Garden; viewpoint)
- ⇒ Igreja da Graça (Graça's church, only outside)
- ⇒ Igreja de S. Francisco (S. Francisco church)
- ⇒ Capela dos Ossos (Bone chapel, to visit inside a fee must be paid per person)



Language: English



Évora 2027, European Capital of Culture is a call for everyone to be an agent of change, taking our vagar to the world: young and old, cultural agents and civil society. Doers and thinkers. Dreamers and the down-to-earth. That's why we say - Take Évora!



Scientific Programme (Conference Time Schedule)

Time	5 th Sept	6 th Sept	7 th Sept	8 th Sept	Time 5 th Sept (afternoon)
9.00-9.45	Registration and Opening Ceremony	(PL5) Ben L. Feringa	(PL9) Robert M. Waymouth	(PL13) Jonathan T. Reeves	
9.45-10.30	(PL1) Karl Anker Jørgensen	(PL6) Joanna Wencel-Delord	(PL10) Teresa M. V. D. Pinho e Melo	(PL14) Yoshiaki Nakao	
	Coffee Break				
11.15-12.00	(PL2) Francesca Paradisi	(PL7) Tanja Weil	(PL11) L.-C. Campeau	(PL15) Kendall N. Houk	
12.00-12:15	(OC1) Arlene G. Corrêa	(OC7) José Ferraz-Caetano	(OC15) Ross Jansen-van Vuuren	Awards and Closing Ceremony	
12:15-12:30	(OC2) Dylan Rigby	(OC8) Paul W. Davies	(OC16) Māris Turks		
Lunch				Social Program	
14.00-14:45	(PL3) Richmond Sarpong	(PL8) Alex M. Szpilman	(PL12) Michael Rack		
14:45-15:00	(OC3) João P. M. António	(OC9) Nieves P. Ramirez	(OC17) Ricardo Mendonça		
15:00-15:15	(OC4) Alexander Ahrens	(OC10) Lukas Enders	(OC18) Klara Bangert		
15:15-15:30	(OC5) Ana L. Cardoso	(OC11) Roberto del Río-Rodríguez	(OC19) Asunción Barbero		
Coffee Break					
16:30-16:45	(OC6) Juliette Martin	(OC12) Alan R. Healy	(OC20) Liam T. Ball		
16:45-17:00	(PL4) Lionel Saudan	(OC13) Laura Cunningham	(OC21) Jens Frackenhohl		
17:00-17:15		(OC14) Carlos Roque Correia	(OC22) Hannah K. Adams		
17:15-18:25	Flash Talks	Flash Talks	Flash Talks (17:15-18:15)		
18:25-19:25	Poster Session 1	Poster session 2	Poster session 3 (18:15-19:15)		
19:30-23:00	Reception party with live Dj		Banquet (20:00-23:30)		

Detailed Scientific Programme:

Tuesday, the 5th of September of 2023

9:00	Registration	
9:30	Opening Ceremony , which includes the Rector of the University of Évora, Professor Hermínia Vasconcelos Vilar (or representative), the president of the Portuguese Chemical Society (SPQ), Professor Joaquim Luís Bernardes Martins de Faria, the director of the Institute for Advanced Studies and Research, University of Évora, Professor Rui Paulo Vasco Salgado (or representative), the director of the School of Science and Technology, University of Évora, Professor Maria Clara Canotilho Grácio (or representative) and the conference chairman, Professor Anthony Burke, University of Coimbra.	
<i>Chairman: Hans-Jürgen Federsel (RISE Research Institutes of Sweden, Sweden)</i>		
9:45	PL 1	Expanding the Borders of Chemical Reactivity <u>Karl Anker Jørgensen</u>
10:30	Coffee Break	
<i>Chairman: Artur Silva (University of Aveiro, Portugal)</i>		
11:15	PL 2	Biocatalysis in flow: when it works and when it doesn't <u>Francesca Paradisi</u>
12:00	OC 1	Synthesis of γ-lactams and Δ^1-pyrroline from chalcones using aziridines and 2H-azirines <u>Arlene G. Corrêa</u>
12:15	OC 2	Towards the Total Synthesis of Mycapolyol E <u>Dylan Rigby</u>
12:30	Lunch	
<i>Chairman: Jorge Salvador (University of Coimbra, Portugal)</i>		
14:00	PL 3	Break-it-to-Make-it Strategies for Chemical Synthesis Inspired by Complex Natural Products <u>Richmond Sarpong</u>
14:45	OC 3	Diazaborines as stable and ROS-responsive linkers: Uncovering a new class of responsive Antibody-Drug Conjugates <u>João P. M. António</u>
15:00	OC 4	Catalytic Disconnection of C–O Bonds in Epoxy Resins and Composites <u>Alexander Ahrens</u>

15:15 **OC 5** **Sustainability meets structural diversity:
exploring the furan-based chemical space**
Ana L. Cardoso

15:30 **Coffee Break**

Chairman: Pedro Cintas (University of Extremadura, Spain)

16:30 **OC 6** **Biocatalysis: a Necessary Tool for Synthetic
Chemist – a Focus on Industrial Applications”**
Juliette Martin

16:45 **PL 4** **Catalysis for the Synthesis of Perfumery
Ingredients**
Lionel Saudan

17:30 **Flash Talks – 1st session**

	Main Auditorium <i>Synthetic Methodology I</i> <i>Chairman: Artur Silva</i> <i>(University of Aveiro, Portugal)</i>	Room 131 <i>PhotoRedox Processes</i> <i>Chairman: Narciso</i> <i>Garrido</i> <i>(University of Salamanca, Spain)</i>	Room 124 <i>Green Processes I</i> <i>Chairman: Jorge</i> <i>Salvador</i> <i>(University of Coimbra, Portugal)</i>
17:30	F 1 <u>Maria João Ferreira</u>	F 7 <u>Pablo Garrido García</u>	F 13 <u>Juliana G. Pereira</u>
17:40	F 2 <u>Sean McCarthy</u>	F 8 <u>Francisco Juliá-Hernández</u>	F 14 <u>Zsuzsanna Fehér</u>
17:50	F 3 <u>Angela Milinkovic</u>	F 9 <u>Adrián Pastor</u>	F 16 <u>Gyula Dargó</u>
18:00	F 4 <u>Bogdan R. Brutiu</u>	F 10 <u>Késsia Andrade</u>	F 17 <u>Giulia Coffetti</u>
18:10	F 5 <u>Aline Makhoutah</u>	F 11 <u>Lukas-Maximilian Entgelmeier</u>	F 18 <u>Raquel Viveiros</u>
18:20	F 6 <u>David Ryan</u>	F 12 <u>Tomasz Wdowik</u>	

18:30 **Poster Session 1**

19:30 **Reception Party**

Wednesday, the 6th of September of 2023

Chairman: Martin Ernst (BASF, Germany)

9:00 **PL 5** **Exploring Chemical Activation**
Ben L. Feringa

9:45 **PL6** **Towards sustainable synthesis of complex molecules via metal-catalyzed or metal-free C-H functionalization**
Joanna Wencel-Delord

10:30 **Coffee Break**

Chairman: Chris Willis (University of Bristol, UK)

11:15 **PL 7** **Polymer Synthesis in Living Systems**
Tanja Weil

12:00 **OC 7** **Explainable Catalytic Epoxide Synthesis Prediction through Machine Learning Models and Descriptive Features**
José Ferraz-Caetano

12:15 **OC 8** **A Nitrenoid Strategy for Efficient N-Heterocycle Synthesis**
Paul W. Davies

12:30 **Lunch**

Chairman: Carlos Afonso (Faculty of Pharmacy, University of Lisbon, Portugal)

14:00 **PL 8** **Discrete Enolonium Species: A New Strategy in Organic Synthesis**
Alex M. Szpilman

14:45 **OC 9** **Asymmetric Synthesis of Trifluoromethylated Propargylic Ethers and Anilines through Multi-Component Reactions**
Nieves P. Ramirez

15:00 **OC 10** **Novel Chiral Imidazopyridine Au(I)-NHC Complexes for Enantioselective Enyne Cycloisomerizations**
Lukas Enders

15:15 **OC 11** **Electrochemical Reactions towards the Synthesis of Distinctive Organic Structures**
Roberto del Río-Rodríguez

15:30 **Coffee Break**

Chairman: Maria João Queiroz (University of Minho, Portugal)

16:30 **OC 12** **A catalytic enantioselective stereodivergent aldol reaction**
Alan R. Healy

16:45 **OC 13** **Scale-up of an Asymmetric sp³-sp² Suzuki-Miyaura Type Reaction**
Laura Cunningham

17:00 **OC 14** **Enantioselective One-pot Cascade Heck-Matsuda Reactions for the Construction of Complex Scaffolds**
Carlos Roque D. Correia

17:15 **Flash Talks – 2nd session**

	Main Auditorium <i>Synthetic Methodology II</i> <i>Chairman: Gesine Hermann</i> <i>(ChiraTecnics, Portugal)</i>	Room 131 <i>Synthetic Methodology III</i> <i>Chairman: Martin Ernst</i> <i>(BASF, Germany)</i>	Room 124 <i>Flow Chemistry/ ElectroSynthesis</i> <i>Chairman: Chris Willis</i> <i>(University of Bristol, UK)</i>
17:15	F 19 <u>Sergey Ryabukhin</u>	F 25 <u>Rūdolfs Bejaunieks</u>	F 30 <u>Américo Alves</u>
17:25	F 21 <u>Tymoteusz Basak</u>	F 27 <u>Rachel Lynch</u>	F 31 <u>Inês S. Martins</u>
17:35	F 22 <u>Enol López</u>	F 29 <u>Nallappan Sundaravelu</u>	F 32 <u>Dmitry Pirgach</u>
17:45	F 23 <u>Miguel Mateus</u>		F 33 <u>Raquel M. Durão</u>
17:55	F 24 <u>Nieves Ledesma</u>		F 34 <u>Mariana Monteiro</u>
18:05			F 35 <u>Miguel A. Bárbara</u>
18:15			F 36 <u>Milene Fortunato</u>

18:25 **Poster Session 2**

Thursday, the 7th of September of 2023

Chairman: Narciso Garrido (University of Salamanca, Spain)

9:00	PL 9	Dynamic Nanomaterials for Gene Delivery: From Chemistry to Biology <u>Robert M. Waymouth</u>
9:45	PL 10	Innovative Chemistry Toward Novel Tetrapyrrolic Macrocycles: Therapy and Imaging of Cancer <u>Teresa M. V. D. Pinho e Melo</u>

10:30 **Coffee Break**

Chairman: Alex Martin Szpilman (Ariel University, Israel)

11:15	PL 11	Changing the World, One Reaction at a Time: The Discovery and Development of Orally Bioavailable Macrocyclic Peptide That Inhibits Binding of PCSK9 to the LDL Receptor <u>L.-C. Campeau</u>
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12:00	OC 15	Directed ortho and Remote Metalation Chemistry for the Formation of Substituted Naphthalenes and Azafluorene Core Liquid Crystals <u>Ross D. Jansen-van Vuuren</u>
12:15	OC 16	Synthesis of allylic systems and heterocycles with highly functionalized olefin side chain from propargyl silanes via 1,2-silyl shift <u>Māris Turks</u>
12:30	Lunch	
<i>Chairman: Gesine Hermann (ChiraTecnics, Portugal)</i>		
14:00	PL 12	Fluorine Chemistry for Agrochemicals <u>Michael Rack</u>
14:45	OC 17	Towards Greener Synthesis: Developing an Environmentally Friendly Process for the Synthesis of an Amide-Containing Drug <u>Ricardo Mendonça</u>
15:00	OC 18	Preparative scale synthesis of α-hydroxylated fatty acids with P450 peroxxygenases <u>Klara Bangert</u>
15:15	OC 19	Recent Approaches Towards the Synthesis of Polysubstituted Heterocyclic Structures <u>Asunción Barbero</u>
15:30	Coffee Break	
<i>Chairman: Maria Manuel Marques (FCT-UNL, Portugal)</i>		
16:30	OC 20	Design and Applications of Bi(V) Reagents for Electrophilic Arylation <u>Liam T. Ball</u>
16:45	OC 21	Transition metal-mediated transformations in Plant Hormone Chemistry: Valuable tools to create new lead structures against abiotic stress in crops <u>Jens Frackenpohl</u>
17:00	OC 22	The Design and Synthesis of Anionic Porphyrins Bearing Chiral Cations and Their Exploration in Catalysis <u>Hannah K. Adams</u>
17:15	Flash Talks – 3 rd session	

Main Auditorium <i>Synthetic Methodology IV</i> <i>Chairman: Hans-Jürgen Federsel (RISE Research Institutes of Sweden, Sweden)</i>		Room 131 <i>Target Oriented Synthesis</i> <i>Chairman: Matthieu Dorbec (Janssen Pharmaceutica)</i>	Room 124 <i>Green (and some other) Processes II</i> <i>Chairman: Maria João Queiroz (University of Minho, Portugal)</i>
17:15	F 37 <u>Dmitriy Volochnyuk</u>	F 43 <u>Soussana Azar</u>	F 49 <u>Luís C. Branco</u>
17:25	F 38 <u>Paula González-Andrés</u>	F 44 <u>Carlos Nieto</u>	F 50 <u>Rafael Gomes</u>
17:35	F 39 <u>Laura F. Peña</u>	F 45 <u>João R. Vale</u>	F 51 <u>Maria Manuel Marques</u>
17:45	F 40 <u>Rocío Bautista</u>	F 46 <u>Vida Malinauskienė</u>	F 52 <u>Yichao Jin</u>
17:55	F 41 <u>Dara Curran</u>	F 47 <u>Daniel Hoffmann</u>	F 53 <u>Alberto Esteban</u>
18:05	F 42 <u>Jasmine Catlow</u>	F 48 <u>Vilija Kederienė</u>	
18:15	Poster Session 3		
20:00	Banquet Dinner		

Friday, the 8th of September of 2023

Chairman: Matthieu Dorbec (Janssen Pharmaceutica)

9:00	PL 13	Practical Organofluorine Chemistry for Large Scale API Synthesis <u>Jonathan T. Reeves</u>
9:45	PL 14	Catalytic Denitrative Transformations <u>Yoshiaki Nakao</u>
10:30	Coffee Break	

Chairman: Luís Branco (FCT-UNL, Portugal)

11:15	PL 15	Computations and Collaborations on Synthetically Important Catalytic Reactions <u>Kendall N. Houk</u>
12:00	Closing Ceremony , which includes the conference chairman, Professor Anthony Burke, University of Coimbra.	
	Social Program	

Plenary Lectures

- PL 1** **Expanding the Borders of Chemical Reactivity**
Karl Anker Jørgensen
- PL 2** **Biocatalysis in flow: when it works and when it doesn't**
Francesca Paradisi
- PL 3** **Break-it-to-Make-it Strategies for Chemical Synthesis Inspired by Complex Natural Products**
Richmond Sarpong
- PL 4** **Catalysis for the Synthesis of Perfumery Ingredients**
Lionel Saudan
- PL 5** **Exploring Chemical Activation**
Ben L. Feringa
- PL 6** **Towards sustainable synthesis of complex molecules via metal-catalyzed or metal-free C-H functionalization**
Joanna Wencel-Delord
- PL 7** **Polymer Synthesis in Living Systems**
Tanja Weil
- PL 8** **Discrete Enolonium Species: A New Strategy in Organic Synthesis**
Alex M. Szpilman
- PL 9** **Dynamic Nanomaterials for Gene Delivery: From Chemistry to Biology**
Robert M. Waymouth
- PL 10** **Innovative Chemistry Toward Novel Tetrapyrrolic Macrocycles: Therapy and Imaging of Cancer**
Teresa M. V. D. Pinho e Melo
- PL 11** **Changing the World, One Reaction at a Time: The Discovery and Development of Orally Bioavailable Macrocyclic Peptide That Inhibits Binding of PCSK9 to the LDL Receptor**
L.-C. Campeau
- PL 12** **Fluorine Chemistry for Agrochemicals**
Michael Rack
- PL 13** **Practical Organofluorine Chemistry for Large Scale API Synthesis**
Jonathan T. Reeves
- PL 14** **Catalytic Denitrative Transformations**
Yoshiaki Nakao
- PL 15** **Computations and Collaborations on Synthetically Important Catalytic Reactions**
Kendall N. Houk

Oral Communications

- OC 1** **Synthesis of γ -lactams and Δ^1 -pyrroline from chalcones using aziridines and 2H-azirines**
Arlene G. Corrêa
- OC 2** **Towards the Total Synthesis of Mycapolyol E**
Dylan Rigby
- OC 3** **Diazaborines as stable and ROS-responsive linkers: Uncovering a new class of responsive Antibody-Drug Conjugates**
João P. M. António
- OC 4** **Catalytic Disconnection of C–O Bonds in Epoxy Resins and Composites**
Alexander Ahrens
- OC 5** **Sustainability meets structural diversity: exploring the furan-based chemical space**
Ana L. Cardoso
- OC 6** **Biocatalysis: a Necessary Tool for Synthetic Chemist – a Focus on Industrial Applications”**
Juliette Martin
- OC 7** **Explainable Catalytic Epoxide Synthesis Prediction through Machine Learning Models and Descriptive Features**
José Ferraz-Caetano
- OC 8** **A Nitrenoid Strategy for Efficient N-Heterocycle Synthesis**
Paul W. Davies
- OC 9** **Asymmetric Synthesis of Trifluoromethylated Propargylic Ethers and Anilines through Multi-Component Reactions**
Nieves P. Ramirez
- OC 10** **Novel Chiral Imidazopyridine Au(I)-NHC Complexes for Enantioselective Enyne Cycloisomerizations**
Lukas Enders
- OC 11** **Electrochemical Reactions towards the Synthesis of Distinctive Organic Structures**
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- OC 15 Directed ortho and Remote Metalation Chemistry for the Formation of Substituted Naphthalenes and Azafluorene Core Liquid Crystals**
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- OC 18 Preparative scale synthesis of α -hydroxylated fatty acids with P450 peroxxygenases**
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Asunción Barbero
- OC 20 Design and Applications of Bi(V) Reagents for Electrophilic Arylation**
Liam T. Ball
- OC 21 Transition metal-mediated transformations in Plant Hormone Chemistry: Valuable tools to create new lead structures against abiotic stress in crops**
Jens Frackepohl
- OC 22 The Design and Synthesis of Anionic Porphyrins Bearing Chiral Cations and Their Exploration in Catalysis**
Hannah K. Adams

Flash Communications

1st Session

Synthetic Methodology I - Main Auditorium

- F 1** **P-C bond Cleavage + H₂ addition in Ruthenium hydride complexes supported by di-tert-butylpyridylphosphine**
Maria João Ferreira
- F 2** **Suzuki-Miyaura coupling using a recycled and reusable homogeneous palladium catalyst**
Sean McCarthy
- F 3** **Mo(VI)=NR/Borane based Frustrated Lewis Pairs: H₂ Activation and Catalytic Reduction of Aldehydes**
Angela Milinkovic
- F 4** **Stereodivergent 1,3-difunctionalisation of unactivated alkenes by charge relocation**
Bogdan R. Brutiu
- F 5** **The quest towards novel synthetic methodologies from nitroarenes for applications in organic electronics**
Aline Makhouloutah
- F 6** **H(O)P(OPh)₂-Promoted Deoxygenative Halogenation of Alcohols**
David Ryan

PhotoRedox Processes - Room 131

- F 7** **Enantioselective Photocatalytic Synthesis of Saturated Bicyclic Scaffolds as Phenyl Bioisosteres**
Pablo Garrido García
- F 8** **Repurposing fluorinated carboxylic acids as fluoroalkylating reagents with Earth-abundant photocatalysts**
Francisco Juliá-Hernández
- F 9** **Improved NO_x removal by visible light photocatalysis through ZnAlEu layered double hydroxides**
Adrián Pastor
- F 10** **Photocatalytic oxidation of biomass-derived heterocycles**
Késsia Andrade
- F 11** **Zwitterionic Acridinium Amidate: A Nitrogen-Centered Photoactive Catalyst Enabling Efficient Hydrogen-Atom Transfer**
Lukas-Maximilian Entgelmeier

- F 12 Red-Light-Induced Functionalizations of Biomolecules**
Tomasz Wdowik

Green Processes I - Room 124

- F 13 Diels Alder reaction of chitin derived furan**
Juliana G. Pereira
- F 14 Depolymerisation of polycarbonate applying silica gel-supported organocatalysts**
Zsuzsanna Fehér
- F 16 MeSesamol, a new, bio-based polar aprotic solvent with versatile applications**
Gyula Dargó
- F 17 Combined chemical and biocatalytic approach for asymmetric one-pot reactions**
Giulia Coffetti
- F 18 Green design of enzyme-inspired dry-powder polymeric catalyst for fast separation processes**
Raquel Viveiros

2nd Session:

Synthetic Methodology II - Main Auditorium

- F 19 Efficient Pd-catalyzed carbonylation of 'benzyl chloride' type compounds – a rare avenue to underrepresented (het)arylacetate platform**
Sergey V. Ryabukhin
- F 21 Cyclic Triel Carbenoids as Auxiliary Ligands for Ruthenium-Based Olefin Metathesis Catalysts**
Tymoteusz Basak
- F 22 C(sp³)-C(sp³) bond formation reactions through organozinc agents**
Enol López
- F 23 Unusual silver complexes bearing N-heterocyclic carbene ligands: synthesis and their application**
Miguel Mateus
- F 24 Diastereoselective synthesis of highly functionalized indolizidine and pyrrolo[1,2-a]azepine derivatives**
Nieves G. Ledesma

Synthetic Methodology III - Room 131

- F 25 Synthesis of Allyl Functionalized Vinyl Silanes from Propargyl Silanes via 1,2-Silyl Migration**
Rūdolfs Beļunieks
- F 27 Phosphonium Ylide-Mediated CO₂ Utilization for the of Synthesis of α,β -Unsaturated Carboxylic Acids**
Rachel Lynch
- F 29 Rhodium-Catalyzed Intermolecular Cross-Cyclotrimerization To Access Selaginulvilins Derivatives and Investigation of Their Medicinal Activity**
Nallappan Sundaravelu

Flow Chemistry/ElectroSynthesis - Room 124

- F 30 Batch and Continuous Flow Synthesis of Novel Spiro- β -Lactams with Antiviral Activity**
Américo J. S. Alves
- F 31 Continuous-Flow Electrochemical Oxidation of Abietanes**
Inês S. Martins
- F 32 Electrochemically Recoverable Homogeneous Catalyst: Genesis, Application and Capture**
Dmitry Pirgach
- F 33 Easy access to functionalized sparteine via electrochemical cyanation of quinolizidine alkaloids**
Raquel M. Durão
- F 34 Synthesis of Imidazolidinones via Palladium-catalysis**
Mariana Crespo Monteiro
- F 35 Photocatalytic modifications of quinic acid derivatives**
Miguel A. Bárbara
- F 36 Accessing Asymmetric Synthesis: Flow Enzymatic Kinetic Resolution of Bicyclic-Aziridines**
Milene A. G. Fortunato

3rd Session:

Synthetic Methodology IV - Main Auditorium

- F 37 Semi-Industrial Synthesis of Diverse Pyrazolines and Cyclopropanes via [3+2]-Cycloaddition between Flow-Generated Diazomethane and Alkenes**
Dmitriy M. Volochnyuk
- F 38 Stereoselective synthesis of an antinociceptive compound by silyl-Prins cyclization**
Paula González-Andrés

- F 39** **Looking for the best selective pathway to obtain cis-2,6-dihdropyran derivatives**
Laura F. Peña
- F 40** **New multitarget neuroprotective drugs with 1,3-cyclohexadien-1-als scaffold**
Rocío Bautista
- F 41** **Phosphine-mediated Reductive Functionalisation of Aldehydes**
Dara Curran
- F 42** **A computational investigation into the Cu-catalysed borylation of α,β -unsaturated compounds**
Jasmine Catlow

Target Oriented Synthesis - Room 131

- F 43** **Thermo-responsive foldamers: Switching from supramolecular polymer to heteroduplex through kinetically trapped foldamers**
Soussana Azar
- F 44** **Virtual Screening of New 2-Phenethylamine Hits Targeting μ -Opioid Receptor**
Carlos Nieto
- F 45** **Total synthesis: From pyridine to (-)-agelastatin A**
João R. Vale
- F 46** **2,5-Substituted-1,3,4-oxadiazoles: Synthesis and Protective Activity Against Oxidative Stress**
Vida Malinauskienė
- F 47** **Development of Readily Accessible Organometallic Capping Reagents for Carbon Labeling of Drugs**
Daniel Vrønning Hoffmann
- F 48** **Synthesis and Biological Studies of Functionalized Bipyrazole Compounds**
Vilija Kederienė

Green (and some other) Processes II - Room 124

- F 49** **Natural Ionic Systems for Homogeneous and Heterogeneous Catalysis**
Luís C. Branco
- F 50** **A New Bio-Based Nitrogen-Rich Furanic Platform Alternative for Lignocellulosic Derived Furfurals**
Rafael F. A. Gomes
- F 51** **Bimetallic Catalysed Synthesis N-heterocycles**
M. Manuel B. Marques

- F 52 Engineering the surface configuration of AgPd alloy catalysts for highly selective oxidation of 5-hydroxymethyl-furfural at room temperature**
Yichao Jin
- F 53 Design of Cocaine Analogues to Treat Psychostimulant use Disorders**
Alberto Esteban

Poster Communications

- P 1** **Blue Light Induced Iron-Catalyzed Alkylation of Ketones with Alcohols**
Nicolas Joly
- P 2** **Synthesis of DHFR inhibitors of *M. avium* and *M. abscessus* via late-stage functionalization of 2,4-dichloropyrimidines**
Ronaldo Aloise Pilli
- P 3** **Selective Catalytic Functionalization of Cavitands**
Laszlo Kollar
- P 4** **Immobilized Cinchonidine-based Catalysts in Deep Eutectic Solvents for Highly Efficient and Sustainable Asymmetric Michael Additions**
Ana C. Amorim
- P 5** **Unveiling the Potential of Phthaloperinones as Active Optoelectronic Compounds for Electronic devices**
Ana C. Amorim
- P 6** **Dual Ni/Organophotoredox Catalysed Allylative Ring Opening Reaction of Oxabenzonornbornadienes and Analogs**
Déborah Paris
- P 7** **Immobilized and Recyclable Catalysts for the Preparation of Deuterium-Labelled Organic Compounds**
Ross D. Jansen-van Vuuren
- P 8** **Ir-Catalysed (Hetero)aryl C-H Functionalisation via N to C Alkyl Transfer**
Erin C. Boddie
- P 9** **Phosphonium Ylide-Mediated CO₂ Utilization for the of Synthesis of α,β -Unsaturated Carboxylic Acids**
Rachel Lynch
- P 10** **H(O)P(OPh)₂-Promoted Deoxygenative Halogenation of Alcohols**
David Ryan
- P 11** **Synthesis of Carbocyclic Boronic Esters through Intramolecular Lithiation-Borylation and Ring Contraction**
Christopher J. Cope
- P 12** **Modular Synthesis of Teraryl-based alpha-Helix Mimetics**
Till Schreiner
- P 13** **Rh(I) Catalysed Regio- and Enantioselective Ring Opening of Cyclopropanes with Boronic Acid Nucleophiles**
Stephen J. Webster
- P 14** **Ortho-Functionalization of Polyhalo-Substituted (Hetero)Aryl Tosylates Using an Integrated Continuous Flow/Batch Protocol**
Yong-Ju Kwon

- P 15** **Synthesis of Benzofused N-Heteropolycycles via Intramolecular Benzyne Cycloadditions using 3-Aminobenzyne Precursors**
Ye-Jin Kong
- P 16** **Continuous Flow Synthesis of N-Sulfonyl-1,2,3-triazoles: Application of Tandem Relay Cu/Rh Dual Catalysis in Microflow Systems**
Min-Jung Lee
- P 17** **Synthesis of γ -aminobutyric acid esters via ring-opening reaction of cyclobutanones**
Ishin Tomiya
- P 18** **The reactivity of C(sp²)-H activated cobalt complexes: a straightforward synthesis of indoles**
Aleksandrs Čižikovs
- P 19** **Cyclic Triel Carbenoids as Auxiliary Ligands for Ruthenium-Based Olefin Metathesis Catalysts**
Tymoteusz Basak
- P 20** **The Design and Synthesis of Anionic Porphyrins Bearing Chiral Cations and Their Exploration in Catalysis**
Hannah K. Adams
- P 21** **De-Acetylative Amination of Acetyl Arenes and Alkanes via Transoximation/Beckmann Rearrangement**
Kengo Hyodo
- P 22** **Metal-catalyzed C-H functionalization of azaarenes with nitroolefins**
Arlene G. Corrêa
- P 23** **N-Aryl-N'-silyldiazenes as Masked Aryl Nucleophiles for the Arylation of Imines and α -Trifluoromethylstyrene Derivatives**
Aliyaah J. M. Rahman
- P 24** **Enantioselective Preparation of Spiro Compounds Using NHC Catalysis**
Ladislav Lóška
- P 25** **Enantioenriched 1,4-Benzoxazepines via Chiral Brønsted Acid Catalyzed Enantioselective Desymmetrization of 3 substituted Oxetanes**
Martin Nigríni
- P 26** **A computational investigation into the Cu-catalysed borylation of α,β -unsaturated compounds**
Jasmine Catlow
- P 27** **New triazine-phosphonate dopants for proton exchange membranes (PEM)**
Fátima C. Teixeira

- P 28** **Next Generation Bioisosteres – Photocatalytic Construction of Azabicycles**
Nicoleta Lazar
- P 29** **Zinc and Alkaline Earth Metal Complexes for the Activation of CO₂**
Dado Rodic
- P 30** **Formal Enone α -Arylation via I(III)-Mediated Aryl Migration/Elimination**
Daniel Kaiser
- P 31** **Enantioselective Photocatalytic Synthesis of Saturated Bicyclic Scaffolds as Phenyl Bioisosteres**
Pablo Garrido García
- P 32** **Hydrogen-bond donor enabled photocatalyzed intramolecular [2+2]-cycloaddition reaction**
Stefania Perulli
- P 33** **Synthesis and characterization of photochemical properties of novel donor-acceptor photosensitizers based on perylene skeleton**
Karolina Socha
- P 34** **Imine hydrosilylation: A theoretical validation through experimental results**
Edgar Silva-Santos
- P 35** **Synthesis of dibenzodiazepinone via Buchwald-Hartwig Amination/Carbonylation**
Amina Moutayakine
- P 36** **Hydroboration of carbon dioxide catalyzed by zinc complexes of borane-tethered bis(pyrazolyl)methane ligands**
Tiago F. C. Cruz
- P 37** **Synthesis of polycyclic compounds containing quaternary carbon centres using tandem carbopalladation/Suzuki-cross coupling reaction and epoxide-arene cyclisation**
Anass Ziari
- P 38** **Design and Synthesis of a Library of Novel Hole Transport Materials based on [2.2]Paracyclophane**
Henrik Tappert
- P 39** **DFT methods as a tool in the search for bifunctional catalysts active in the dual process of polymerization and depolymerization**
Edyta Nizioł
- P 40** **Photocatalytic Generation of Trifluoromethyl Nitrene and its Use in Alkene Aziridination**
Norbert Baris
- P 41** **Synthesis of 5H-pyrazino[2',3':4,5]pyrrolo[3,2-d]pyrimidin-4-amine as a core structure for potential antivirals**
Luca Julianna Tóth

- P 42 Sequential Reactivity of Molecular Flavin Catalysts**
Alexandra Walter
- P 43 Decarboxylative-Carbonylative Nickel-Catalyzed Cross-Coupling for the Efficient Isotopic Labeling of Aryl-Alkyl Ketones**
Vitus J. Enemærke
- P 44 N-Heterocyclic Carbenes as Versatile Tool for Molecular Surface Modification**
Arne Nalop
- P 45 Photoredox-Catalyzed Defluorinative Functionalizations of Polyfluorinated Aliphatic Amides and Esters**
Corinna Heusel
- P 46 Cobalt-pincer complexes based on triazine backbone - application in the synthesis of organometalloid compounds**
Dariusz Lewandowski
- P 47 Unique synthesis of new heterodimeric zinc complexes**
Aleksandra Marszałek-Harych
- P 48 Palladium-Catalyzed C(sp³)-H Arylation Of Pentacyclic Triterpenoids**
Vladislavs Kroškins
- P 49 Post-Synthesis Strategies to Prepare Mesostructured and Hierarchical Silicate Catalysts for Olefin Epoxidation**
Diana M. Gomes
- P 50 Application of N-Amino pyridinium salts in photochemistry**
Kitti Franciska Szabó
- P 51 Suzuki-Miyaura coupling using a recycled and reusable homogeneous palladium catalyst**
Sean McCarthy
- P 52 The Use of Azide-Tetrazole Equilibrium in the Modification of Fused Pyrimidines**
Irina Novosjolova
- P 53 Mechanochemical borylation of aryl diazonium salts promoted by sodium chloride**
Samuel Andrejčák
- P 54 Synthetic Pathways Toward Designed Purine Derivative for the Photo-Catalysis**
Aleksejs Burcevs
- P 55 Azide-Tetrazole Equilibrium Driven Reactions of Fused Diazido Pyrimidines and Characterization of Tautomerism Therein**
Kristaps Leškovskis
- P 56 Pyridine-2-carboxylate Palladacycle Catalyzed Addition of Arylboronic Acids to Electron-deficient Alkenes**
Yuki Izumiya

- P 57 Synthesis of Chiral 3-Allyl-isoindolinone Derivatives via Optical Resolution**
Ryota Ozawa
- P 58 Redox-active esters as key intermediates in the synthesis of sulfur-derivatives of oseltamivir**
Barbora Zahradníková
- P 59 Development of Readily Accessible Organometallic Capping Reagents for Carbon Labeling of Drugs**
Daniel V. Hoffmann
- P 60 Synthesis and Photophysical Properties of Phosphorescent Purine-Iridium Complexes**
Armands Sebris
- P 61 Anion-Binding Catalyzed Asymmetric Dearomatization of 4-Oxy-quinolinium Salts**
Martin Aleksiev Pakovski
- P 62 Switching from Ionic to Radical Type Chemistry: Radical NHC-Catalysis Enables the Regiodivergent C–H Acylation of (Hetero)Arenes**
Jannik Reimler
- P 63 Masked malondialdehydes - efficient synthons for functionalized heterocycles**
Sergey Ryabukhin
- P 64 Beyond the noble-metal-contained catalytic systems - solutions for Pd-crisis**
Dmitriy M. Volochnyuk
- P 65 Evaluation of Potential Small and Macromolecular Anti-SARS-CoV-2 Agents**
Vitalijs Rjabovs
- P 66 EnTdecker: Predicting excited state properties of organic molecules to accelerate substrate discovery for energy transfer catalysis**
Leon Schlosser
- P 67 C-H Amination of Pentacyclic Triterpenoids**
Jevgenija Luginina
- P 68 Catalytic Disconnection of C–O Bonds in Epoxy Resins and Composites**
Alexander Ahrens
- P 69 Borylative Transition-Metal Free Cross Couplings with Vinyl Iodides**
Gesa Seidler
- P 70 An efficient alcoholysis of primary amides**
Anton Mastitski

Synthesis and Photophysical Properties of Phosphorescent Purine-Iridium Complexes

Armands Sebris, Kaspars Traskovskis, Irina Novosjolova, Māris Turks

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There is ongoing research towards more efficient emitters in organic light-emitting diodes (OLED), and especially for structures, that emit light in the blue region. Highly efficient emitters can be achieved using phosphorescent transition metal complexes, that can utilize excited triplet states for emission. To the best of our knowledge, there are only 2 publications that have examined the photophysical properties of iridium complexes with purine carbenes.¹ So further research in this field is necessary to yield optimized emitters for OLEDs.

The purine ligand was prepared from a functionalized pyrimidine via *de novo* synthesis. *Mer* isomer **1** was selectively formed in a AgOAc mediated reaction, while *fac* isomer **2** was prepared in an acid catalyzed isomerization.² XRD structures were achieved to prove the identity of both isomers (**Figure 1**). Both isomers emitted blue light, with *mer* isomer showing a bathochromic shift compared to *fac* isomer. Emission also exhibited a bathochromic shift, when comparing PMMA doped solid state to DCM solution. Quantum yields in PMMA reached up to 100%.

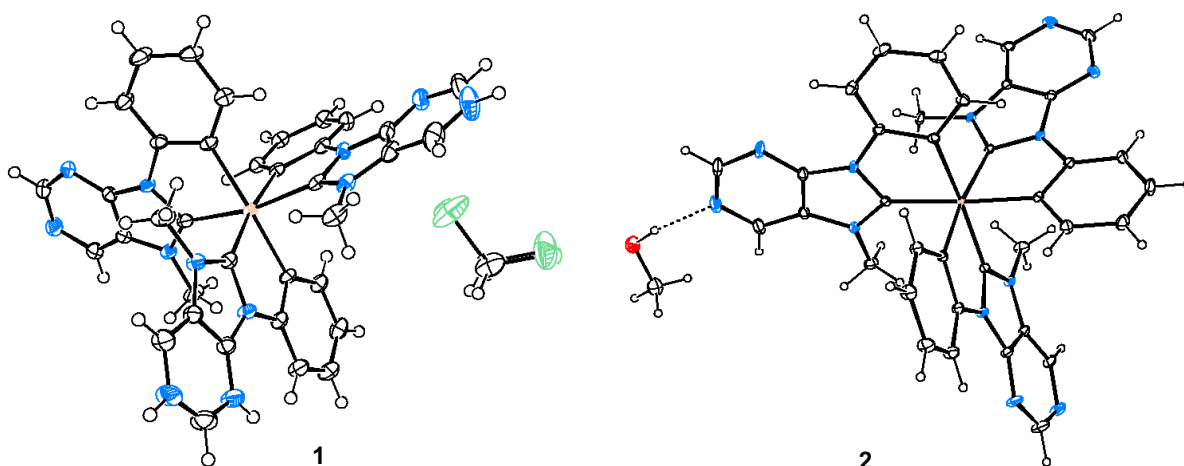


Figure 1: XRD structures of *mer* **1** and *fac* **2** purine-iridium complexes.

Acknowledgements: This work was supported by the Latvian Council of Science grant No. LZP-2020/1-0348. Dr. phys. A. Mishnev is acknowledged for X-ray analysis.

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