

# 8<sup>TH</sup> INTERNATIONAL CONFERENCE ON MULTICOMPONENT REACTIONS AND RELATED CHEMISTRY



September 6 – 8, Burgos, Spain



Dear All,

On behalf of the Local Organizing Committee of the 8th International Conference on Multicomponent Reactions and related Chemistry, we send our warmest regards to the scientific community that will be participating at symposium which will take place in Burgos, between September 6th an 8<sup>th</sup>, 2023.

The Organizing Committee, in close collaboration with the Scientific Committee, has prepared an attractive program, addressing cutting edge topics with especial emphasis in young scientists. In this respect, we want to publicly thank the generosity of senior researchers for facilitating this transition, which we believe will have a very positive impact in the future of the field.

The conference will take place in a unique environment, the Hospital del Rey of the University of Burgos, a historic building and former pilgrim's hospital on the Camino de Santiago.

We would like you to share your excellent research in Burgos, and to enjoy the welcoming spirit of our city.

We are looking forward to seeing you in Burgos

Prof. María García Valverde

Chair of the Local Organizing Committee



#### **Conference Venue**

Aula Romeros Facultad de Derecho Universidad de Burgos Hospital del Rey s/n 09001 Burgos Spain

#### How to arrive

Located a 20-minute walk from the city center, along the river. By Bus: Lines 7 or 12. UBU direction. Get off at the stop Hospital del Rey (See Burgos Bus Map below)

#### Congress web

www2.ubu.es/mcr2023

#### Registration

Wednesday September 6 from 8:00 a.m. at the conference venue.

#### **Oral presentations**

Conference room will be equipped with PC computer with HDMI output, Windows 10 professional operating system, and Microsoft Office 365.

#### Certificates

Certificates of attendance and participation will be sent after the Meeting, by email. The participation certificate will be sent to the corresponding contact author.

#### **Coffee Breaks**

Coffee breaks will take place in Patio Romeros of the Hospital del Rey.

#### **Lunch Breaks**

Lunch breaks will take place in the Cafeteria of the Hospital del Rey.

#### **Conference Dinner**

The conference dinner will take place at the Hotel Rice Palacio de los Blasones (C/ Fernán González, 10, 09003 Burgos) on Thursday September 7 at 20:00.



# **CONFERENCE VENUE**





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HOSPITAL DEL REY



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HOTEL RICE BULEVAR

HOTEL AZOFRA

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Hotel Rice Reyes Católicos

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BURGOS CATHEDRAL

C.H HOTEL AZOFRA







September 6-8, Burgos, Spain

# SCIENTIFIC COMMITTEE

Rodolfo Lavilla. Universitat de Barcelona Romano V. A. Orru. Maastricht University Ludger A. Wessjohann. Leibniz Institute of Plant Biochemistry Erik Van der Eyken. KU Leuven María García Valverde. Universidad de Burgos

# ORGANIZING COMMITTEE

María García Valverde. Universidad de Burgos Rodolfo Lavilla. Universitat de Barcelona Ouldouz Ghashghaei. Universitat de Barcelona Roberto Quesada Pato. Universidad de Burgos Israel Carreira Barral. Universidad de Burgos Pau Nadal. Universitat de Barcelona



### PLENARY LECTURES

PL-1. Thomas J. J. Müller. Heinrich-Heine-University. Germany

FUNCTIONAL CHROMOPHORES BY MULTICOMPONENT REACTIONS

PL-2. Géraldine Masson. Paris-Saclay University. France

CATALYTIC MULTICOMPONENT VICINAL DIFUNCTIONALIZATION OF ALKENES

PL-3. Eelco Ruijter. Vrije Universiteit Amsterdam. The Netherlands

LEVERAGING ISOCYANIDE CHEMISTRY FOR DRUG DISCOVERY AND PRODUCTION

PL-4. Paolo Melchiorre. University of Bologna. Italy

PHOTOCHEMISTRY & ORGANOCATALYSIS: NEW RADICAL OPPORTUNITIES

PL-5. Gonçalo Bernardes. University of Cambridge. United Kingdom

TRANSLATIONAL CHEMICAL BIOLOGY



# **INVITED LECTURES**

IL-1. Andrea Basso. University of Genova. Italy

KETENES AS VERSATILE BUILDING BLOCKS IN MULTICOMPONENT REACTIONS

IL-2. Ana Mallo-Abreu (Sotelo's group). University of Santiago de Compostela. Spain

EVOLUTIONARY APPROACHES FOR THE MCR-ASSITED DISCOVERY AND OPTIMIZATION OF ADENOSINE RECEPTOR ANTAGONISTS

IL-3. Wenhao Hu. Sun Yat-sen University. China

ENANTIOSELECTIVE MULTICOMPONENT REACTIONS VIA TRAPPING OF REACTIVE INTERMEDIATES

IL-4. Martín Fañanás-Mastral. University of Santiago de Compostela. Spain

CATALYTIC STEREOSELECTIVE HYDROCARBON DIFUNCTIONALIZATION

IL-5. Carlos Fernández Marcos. University of Extremadura. Spain

REACTIVE INTERMEDIATES IN MULTICOMPONENT REACTIONS OF ISOCYANIDES: THE CASES OF THE ENOL-UGI CONDENSATION AND CYCLOADDITION PROCESSES IN TANDEM

IL-6. Gian Cesare Tron. University of Piemonte Orientale. Italy

OLD DOG, NEW TRICKS. ISOCYANIDE: FROM STRATEGIC FUNCTIONAL GROUP FOR NOVEL MULTICOMPONENT REACTIONS TO INNOVATIVE PHARMACOPHORIC GROUP IN MEDICINAL CHEMISTRY

IL-7. Laurence Grimaud. Sorbonne University. France

ELECTROOXIDATIVE ISOCYANIDE-BASED REACTIONS

IL-8. Upendra Kumar Sharma. KULeuven. Belgium

PHOTOCATALYZED MULTICOMPONENT REACTIONS: HARNESSING LIGHT FOR EFFICIENT AND SUSTAINABLE SYNTHESIS

IL-9. Svetlana Tsogoeva. University of Erlangen-Nürnberg. Germany

METAL-FREE MULTI-STEP DOMINO REACTIONS



IL-10. Bernhard Westermann. Leibniz Institute for Plant Biochemistry. Germany

PHYTOCERAMIDES - SCAFFOLD DIVERSIFICATION AND APPLICATIONS AS ADJUVANTS

IL-11. Wei Zhang. University of Massachusetts. USA

INTEGRATED ONE-POT STEPWISE SYNTHESIS AND ORGANOCATALYSIS



# ORAL COMMUNICATIONS

# OC-1. Rocío Gámez-Montaño. University of Guanajuato. Mexico

MECHANOCHEMICAL IMCR and IMCR-POST TRANSFORMATION DOMINO STRATEGIES: TOWARDS THE SUSTAINABLE DOS OF DIPEPTIDE-LIKE AND HETEROCYCLIC PEPTIDOMIMETICS

OC-2. Ahmad Shaabani. Shahid Beheshti University. Iran

MATERIALS FUNCTIONALIZATION AND MODIFICATION *VIA* MULTICOMPONENT REACTIONS AND THEIR APPLICATIONS

OC-3. Pau Nadal. University of Barcelona. Spain

DISCOVERY OF NEW MULTICOMPONENT PROCESSES THROUGH CHARTING OF THE CHEMICAL REACTION SPACE

OC-4. Maxime R. Vitale. Sorbonne University. France

PHOTOREDOX-CATALYZED PSEUDO-4-COMPONENT ALKYLATIVE AMIDINATION OF ALKENES

OC-5. Xabier del Corte. University of the Basque Country. Spain

ENANTIOSELECTIVE MULTICOMPONENT REACTION FOR THE SYNTHESIS OF UNSATURATED  $\gamma$ -LACTAM DERIVATIVES AND THEIR SYNTHETIC APPLICATIONS

OC-6. Tullio Crovetto. University of Genova. Italy

HIGHLY CONJUGATED LUMINESCENT FURO[2,3-*c*]ISOQUINOLINES AS FLUOROPHORES BY COUPLING THE UGI REACTION WITH A Pd(0)-CATALYZED DOUBLE CYCLIZATION

OC-7. Javier Gómez-Ayuso. University of Burgos. Spain

SYNTHESIS OF NOVEL TETRAHYDRONAPHTHOAZETIDINONES, 2,5-DIOXO-1,4-METHANO-BENZOAZEPINES AND 3-HYDROXYPYRROLIDINONES THROUGH COPPER-ASSISTED POST-UGI DOMINO SEQUENCES

OC-8. Jordy M. Saya. Maastricht University. The Netherlands

ENHANCING THE SPEED OF THE PASSERINI REACTION



OC-9. Dayana Alonso. University of Havana. Cuba

MULTICOMPONENT DERIVATIZATION OF THE CEMADOTIN SKELETON – IN SILICO STUDY AND IN VITRO CYTOTOXIC ACTIVITY

OC-10. Tetiana Pavlovska. University of Chemistry and Technology Prague. Czech Republic

POWERFUL FLAVIN PHOTOCATALYSTS VIA THREE-COMPONENT REACTION: SYNTHESIS AND APPLICATION

OC-11. Carlos Kleber Zago de Andrade. University of Brasilia. Brasil

GREENER SYNTHESIS AND PHYTOTOXICITY SCREENING OF GBB-3CR ADDUCTS

OC-12. Anita Vißers. Heinrich-Heine-University. Germany

SUSTAINABLE ONE-POT SYNTHESES OF FUNCTIONAL DYES

OC-13. Marine Pinaud. University of Paris Est. France

MIXED ALIPHATIC ORGANOZINC REAGENTS AS NON-STABILIZED CSP3-NUCLEOPHILES IN MULTICOMPONENT REACTIONS



# POSTER COMMUNICATIONS

PO-1. Carlos Rodríguez-Garcia. University of Santiago de Compostela. Spain

A BIGINELLI-BASED APPROACH FOR THE OPTIMIZATION OF POTENT AND SELECTIVE  $\mathsf{A}_1\mathsf{AR}$  ANTAGONISTS

PO-2. Tuvshinjargal Budragchaa. Leibniz-Institute of Plant Biochemistry. Germany

SYNTHESIS, MODIFICATION AND BIOLOGICAL EVALUATION OF  $\gamma\text{-}OXOCROTONIC$  ACID DERIVATIVES

PO-3. Pablo López. University of Santiago de Compostela. Spain

UGI-BASED ASSEMBLY OF OSELTAMIVIR DERIVATIVES

PO-4. Aitor García-Rey. University of Santiago de Compostela. Spain

A MULTICOMPONENT APPROACH ENABLED THE DISCOVERY OF SUBTYPE SELECTIVE AND BIASED D2 BITOPIC LIGANDS

PO-5. Erik V. Van der Eycken. KU Leuven. Belgium

GOLD(I)-CATALYZED INTRAMOLECULAR BICYCLIZATION: DIVERGENT CONSTRUCTION OF QUINAZOLINONE AND AMPAKINE ANALOGUES

PO-6. Leonardo González Ceballos. University of Havana. Cuba

A RADICAL MULTICOMPONENT APPROACH FOR THE SITE-SELECTIVE MODIFICATION OF PEPTIDES

PO-7. Iván Rodríguez-Pampín. University of Santiago de Compostela. Spain

MULTICOMPONENT-ASSISTED DISCOVERY OF MULTITARGET DRUGS: DESIGN, OPTIMIZATION AND *EX VIVO* TUMOR ASSAYS

PO-8. Rocío Gámez-Montaño. University of Guanajuato. Mexico

MECHANOCHEMICAL IMCR AND IMCR-POST TRANSFORMATION DOMINO STRATEGIES: TOWARDS THE SUSTAINABLE DOS OF DIPEPTIDE-LIKE AND HETEROCYCLIC PEPTIDOMIMETICS



# PO-9. Ana Mallo-Abreu. University of Santiago de Compostela. Spain

NITROGEN-WALK APPROACH: AN EVOLUTIONARY BIGINELLI-BASED APPROACH TO EXPLORE BIOISOSTERIC REPLACEMENTS IN A2B ADENOSINE RECEPTOR ANTAGONISTS

# PO-10. Rocío Gámez-Montaño. University of Guanajuato. Mexico

SYNTHESIS OF *BIS*-AMIDES VIA UGI REACTION: FUNCTIONALIZATION OF MASTICADIENONIC ACID, A TRITERPENOID ISOLATED FROM FRUIT PEDUNCLES OF *PISTACIA MEXICANA* 

PO-11. Hugo Fojo-Carballo. University of Santiago de Compostela. Spain

BIGINELLI-INSPIRED SCAFFOLD HOPPING APPROACHES FOR THE OPTIMIZATION OF  $\mathsf{A}_{2\mathsf{B}}$  ANTAGONISTS

PO-12. Antonio Andújar-Arias. University of Santiago de Compostela. Spain

UGI-BASED ASSEMBLY OF PERIPHERAL SELECTIVE RIMONABANT ANALOGUES

PO-13. David Reza. University of Santiago de Compostela. Spain

UGI-BASED APPROACHES ENABLED THE DISCOVERY OF A NOVEL CLASS OF CANNABINOID RECEPTOR LIGANDS

PO-14. Gereon Hendrik Schmitz. Heinrich-Heine-University Düsseldorf. Germany

PREPARATION OF 3-ACYLPYRROLES AND SULFENYLATED ENAMINONES VIA FOUR-COMPONENT ONE POT SYNTHESES

PO-15. Giovanni Graziano. University of Santiago de Compostela. Spain

DISCOVERY AND OPTIMIZATION OF NEW  $\mathsf{CB}_2\mathsf{R}$  selective biased agonists as potent anti-inflammatory agents

PO-16. Larissa K. E. Hinz. Heinrich-Heine-University Düsseldorf. Germany

CONVERGENT ONE-POT SYNTHESIS OF INDOLO[3,2-*a*]PHENAZINE DERIVATIVES – INVESTIGATING MEDICINAL AND PHOTOPHYSICAL PROPERTIES

PO-17. Lucia González-Pico. University of Santiago de Compostela. Spain

BIGINELLI REACTION ENABLED THE IDENTIFICATION OF A2B AND DUAL A2B/A2A ANTAGONISTS FOR CANCER IMMUNOTHERAPY



PO-18. Luca Banfi. University of Genova. Italy

PRELIMINARY STUDIES ON MCRs USING LEVOGLUCOSENONE AS BIO-BASED STARTING MATERIAL

PO-19. Cristina Martini. University of Genova. Italy

THE USE OF NEW ISOCYANIDES IN THE GBB THREE-COMPONENT REACTION FOR THE SYNTHESIS OF NOVEL ORGANIC FLUOROPHORES

PO-20. Dario Miranda-Pastoriza. University of Santiago de Compostela. Spain

UGI-BASED EXPLORATION OF NON-ORTHOSTERIC INTERACTIONS WITH A SERIES OF POTENT A3 ANTAGONISTS

PO-21. Muhammad Idham Darussalam Mardjan. Gadjah Mada University. Indonesia

ONE-POT SYNTHESIS OF ISOINDOLIN-1-ONES UNDER ULTRASONIC IRRADIATION

PO-22. Francesca Brunelli. University of Piemonte Orientale. Italy

THE ISOCYANIDE AS NOVEL PHARMACOPHORIC GROUP: ONE-POT SYNTHESIS OF POTENT ANTIBACTERIAL AGENTS USING MULTICOMPONENT REACTIONS

PO-23. Maryna Kornet. Heinrich-Heine-University Düsseldorf. Germany

 $\alpha\text{-}\mathsf{KETOGLUTARIC}$  ACID IN MULTICOMPONENT REACTIONS

PO-24. José Luis Ramiro. University of Extremadura. Spain

HETEROCYCLIC SCAFFOLD SYNTHESIS THROUGH ENOL-UGI/REDUCTION/CYCLISATION

PO-25. Lucía Campos-Prieto. University of Santiago de Compostela. Spain

A1AR ANTAGONISTS WITH ENANTIOSPECIFIC RECOGNITION ASSEMBLED THROUGH A BIGINELLI-BASED APPROACH

PO-26. Carlos Cámara Herrero. University of Burgos. Spain

UDC STRATEGY IN THE SYNTHESIS OF PYRROLOPIPERAZINONES

PO-27. Sandra Ortigueira-Noya. University of Santiago de Compostela. Spain

MCR-ASSISTED DISCOVERY AND OPTIMIZATION OF NOVEL A<sub>2A</sub> ADENOSINE RECEPTOR ANTAGONISTS FOR CANCER IMMUNOTHERAPY



# PO-28. Thaissa Pasquali F. Rosalba. University of Brasilia. Brasil

DESIGN AND SYNTHESIS OF LIPID PEPTOID NANOPARTICLES FOR TARGETED DRUG DELIVERY VIA UGI REACTION

## PO-29. Tullio Crovetto. University of Genova. Italy

THE USE OF UGI FOUR-COMPONENT REACTION COUPLED WITH A Pd0-CATALYSED DOMINO PROCESS FOR THE SYNTHESIS OF NOVEL HIGHLY CONJUGATED ORGANIC FLUOROPHORES

#### PO-30. Daniël S. Verdoorn. University of Antwerp. Belgium

A COBALT MEDIATED NITRENE TRANSFER AZA-WITTIG CASCADE REACTION TO ACCESS 1,3,4-OXADIAZOLE SCAFFOLDS

#### PO-31. Beatriz González-Saiz. University of Burgos. Spain

SYNTHESIS OF HIGHLY FUNCTIONALIZED HETEROCYCLES BY UGI/NUCLEOPHILIC SUBSTITUTION/RING EXPANSION SEQUENCES

#### PO-32. Carme Masdeu. University of the Basque Country. Spain

PREPARATION OF MORE LIPOPHILIC ANTIMYCOLATA AGENTS BY MODIFICATION OF KNOWN ANTIBIOTICS THROUGH MULTICOMPONENT REACTIONS

# PO-33. Ángela Trejo. University of the Basque Country. Spain

PREPARATION OF NOVEL TOPOISOMERASE I INHIBITORS THROUGH MULTICOMPONENT REACTIONS

PO-34. Endika Martín-Encinas. University of the Basque Country. Spain

SYNTHESIS AND BIOLOGICAL EVALUATION OF FUSED HETEROCYCLES DERIVATIVES AS HUMAN TOPOISOMERASE I INHIBITORS

PO-35. Julene Allende. University of the Basque Country. Spain

THE JOULLIÉ-UGI THREE-COMPONENT REACTION AS A SYNTHETIC TOOL FOR THE DIASTEROSELECTIVE PREPARATION OF HIGHLY FUNCTIONALIZED *N*-ACYLAZIRIDINE DERIVATIVES

PO-36. Daniel Preschel. Vrije Universiteit Amsterdam. The Netherlands

MULTICOMPONENT SYNTHESIS OF THE SARS-COV-2 MAIN PROTEASE INHIBITOR NIRMATRELVIR



PO-37. Brendan Horst. Vrije Universiteit Amsterdam. The Netherlands

TOTAL SYNTHESIS OF COMPLEX INDOLE ALKALOIDS BY A NITROARYL TRANSFER CASCADE REACTION



Wednesday Sept 6		Thursday Sept 7		Friday Sept 8		
8:00-8:30 h	Registration	MARCACCINI MEMORIAL LECTURE				
8:30-9:00 9:00-9:50	Official Opening PL-1 (Müller)	8:30-9:20	PL-3 (Ruijter)	8:30-9:20	PL-5 (Bernardes)	
		9:30-10:00	IL-5. Marcos	9:30-10:00	IL-10. Westermann	
10:00-10:30	IL-1. Basso	10:05-10:35	IL-6. Tron	10:05-10:20	OC-11	
			OC-6	10:25-10:40	OC-12	
10:35-10:50	0C-1	10:40-10:55		10:45-11:00	OC-13	
11:00-11:30		COFFEE BREAK				
11:30-12:00	IL-2. Mallo-Abreu (Sotelo's group)	11:30-12:00	IL-7. Grimaud	11:40-12:10	IL-11. Zhang	
12:10-12:25	OC-2	12:10-12:25	OC-7			
12:30-12:45	OC-3	12:30-12:45	OC-8	12:20-13:00	Closing remarks	
12:50-13:05	OC-4	12:50-13:05	OC-9			
13:10-14:40	LUNCH BREAK					
14:50-15:40	PL-2 (Masson)	14:50-15:40	PL-4 (Melchiorre)	PL: Plenary lectures IL: Invited Lectures OC: Oral Communications		
15:50-16:20	IL-3. Hu	15:50-16:20	IL-8. Sharma			
16:30-17:00	IL-4. Fañanás	16:30-17:00	IL-9. Tsogoeva			
17:10-17:25	OC-5	17:10-17:25	OC-10			
17:30-19:30	POSTER SESSION and DRINKS	Cultural Visit		]		
		20:00-23:00	CONFERENCE DINNER			



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