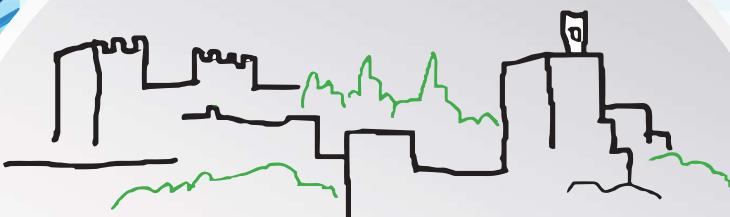


GRANADA

Book of Abstracts



February 19-21, 2020

V GEQB ChemBio Group Meeting

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February 19-21, 2020

V GEQB ChemBio Group Meeting

PROGRAMME

WEDNESDAY, February 19th, 2020

09:00-10:45 REGISTRATION + COFFEE

10:45-11:00 GEQB – OPENING

Mario Delgado, IPBLN-CSIC, Granada, Spain

Juan Carlos Morales Sánchez, IPBLN-CSIC, Granada, Spain

11:00-13:30 SESSION 1

Chair: Juan Carlos Morales Sánchez

11:00-11:45

Plenary Lecture (sponsored by "Molecules", MDPI)

A chemistry-based multidisciplinary strategy to semi-synthetic glycovaccines: from concept to first-in-human study and more in the context of *Shigella*

Laurence A. Mular, Institute Pasteur, France

11:45-12:15 **Invited Lecture**

Impact of Biophysical Techniques on Drug Discovery

Juan Félix Espinosa, Lilly, Madrid, Spain

12:15-12:45 **Invited Lecture**

Turning stem cells into a medicine

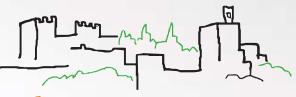
Mario Delgado, IPBLN-CSIC, Granada, Spain

12:45-13:15 **Oral Communications**

OC1. Glycodendropeptides as potential synthetic vaccines against allergy
Javier Rojo, IIQ-CSIC, Seville, Spain

OC2. Development of new streamlined saponin vaccine adjuvants: molecular-level insights into saponin conformation correlating with adjuvant activity

Alberto Fernández-Tejada, Cicbiogune, Bilbao, Spain



February 19-21, 2020

V GEQB ChemBio Group Meeting

13:15-13:30 Flash Communications

FC1. Pablo Valverde, NMR Studies of the specific interaction of DC-SIGN with the blood group A/B antigens

FC2. Beatriz Fernández de Toro, Avenues to characterize the interactions of extended N-glycans with proteins by NMR spectroscopy: the influenza hemagglutinin case

FC3. Manuel González Cuesta, Enzyme regulators with self-delivery capabilities

13:30-15:00 LUNCH

15:00-16:30 SESSION 2

Chair: Rosario Sánchez Martín

15:00-15:30 Invited Lecture

Multi-Scale Approaches to Computer-Assisted Enzyme Design

Gonzalo Jiménez-Oses, CICBiogune, Bilbao, Spain

15:30-16:00 Invited Lecture

Efficient and Sustainable Synthesis of Muramic and Glucuronic acid Glycodendrimers as Dengue Virus Antagonists

María José Hernáiz Gómez, Universidad Complutense, Madrid, Spain

16:00-16:15 Oral Communication

OC3. sp2-Iminosugar glycolipid mimetics as immunoregulatory agents

Elena M. Sánchez, University of Seville, Spain

16:15-16:30 Flash Communications

FC4. Alejandra Matamoros Recio, Computational approaches to the structure and activation mechanism of Toll-like receptor 4

FC5. José Antonio Laz-Ruiz, TDesign and development of novel nanodevices for biomedical applications

FC6. María Pia Lenza, Deciphering the N-glycan profile and interactions of FcεRIα by NMR

16:30-17:00 COFFEE BREAK + POSTER SESSION 1



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17:00-18:30

SESSION 3

Chair: Ignacio Alfonso

17:00-17:30 **Invited Lecture**

Designing the 3D microenvironment of cells for the bioengineering of humanized tissues

Joao Mano, University of Aveiro, Portugal

17:30-18:00 **Invited Lecture**

Discovery of Novel Spirocycles as Inhibitors of the Mitochondrial Permeability Transition Pore Opening for the Treatment of Myocardial Reperfusion Injury

Delia Preti, University of Ferrara, Italy

18:00-18:15 **Oral Communication**

OC4. Interaction of amyloid- β with functionalised gold nanoparticles

Patrick Gámez, University of Barcelona, Spain

18:15-18:30 **Flash Communications**

FC7. Reyes Núñez Franco, Computational prediction of activity-enhancing mutations by allosteric networks optimization

FC8. María Dolores Moya Garzón, Development of salicylate derivatives with double GO/LDHA inhibitory activity as pharmacological approach for the treatment of primary hyperoxaluria type 1

FC9. Marta Pazo Pascual, Lipid responsive helical oligoalanines for cell penetration

18:30-19:00

MEETING – GEQB



February 19-21, 2020

V GEQB ChemBio Group Meeting

THURSDAY, February 20th, 2020

09:00-11:00

SESSION 4

Chair: José Luis Mascareñas

09:00-09:45 **Plenary Lecture** (*sponsored by "Pharmaceuticals", MDPI*)

The Chemistry-medicine continuum: approaches to HIV/AIDS eradication and to enhanced immuno-therapy

Paul Wender, Stanford University, USA

09:45-10:15 **Invited Lecture**

To be announced

María Jesús Vicent, Centro de Investigación Príncipe Felipe, Valencia, Spain

10:15-10:45 **Invited Lecture**

Structural Studies of Weak Protein-Ligand Complexes by NMR: Novel Saturation Transfer Difference (STD) NMR Approaches

Jesús Angulo, Universidad de Sevilla , Spain

10:45-11:00 **Flash Communications**

FC10. Javier Valverde Pozo, A fluorescence ICT sensor for aminopeptidase detection in live cells

FC11. Joan Miguel-Ávila, Transition Metal Promoted Cycloadditions in Biologic Media

FC12. Esther Jiménez Moreno, Acetals as acid-sensitive cleavable linkers for the design of antibody-drug conjugates

11:00-11:30

COFFEE BREAK + POSTER SESSION 1

11:30-13:30

SESSION 5

Chair: María Jesús Vicent

11:30-12:00 **Invited Lecture**

Bio-inspired Materials Based on Simple Peptidic Derivatives

Beatriz Escuder, Universitat Jaume I, Castellón, Spain

12:00-12:30 **Invited Lecture**

Nature-inspired DNA-based nanodevices for diagnostic and drug-delivery applications

Francesco Ricci, University of Rome, Italy



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Química Terapéutica

12:30-13:00 **Invited Lecture** (sponsored by SEQT)

Development of synthetic Toxin-Antitoxin-based therapeutic systems for cancer treatment

Guillermo de la Cueva, Bionand, Spain

13:00-13:30 **Oral Communications**

OC5. Chemo-Enzymatic Total Synthesis of Sorbicillinoid Natural Products

Anna Sib, ICIQ Tarragona, Spain

OC6. Applying dynamic chemistry for miR-21 direct detection and quantification

Antonio Delgado -González, University of Granada, Spain

13:30-15:00

LUNCH

15:00-16:30

SESSION 6

Chair: Óscar Millet

15:00-15:30 **Invited Lecture** (*Young Investigator GEQB Award*)

Supramolecular Chemistry Synthesizing Artificial Biology

Javier Montenegro, CIQUS, Santiago de Compostela, Spain

15:30-16:15 **Oral Communications**

OC7. Dendrimers as a powerful tool in biomedicine. Applications in tissue regeneration processes and as biomarkers

Yolanda Vida, University of Málaga, Spain

OC8. Ruthenium-catalyzed redox isomerizations inside living cells

Christian Vidal, CIQUS, Santiago de Compostela, Spain

OC9. Fighting Resistances: Photoswitchable Antimicrobials Fully Operated under Visible Light

Xavier Just-Baringo, IRB, Barcelona, Spain

16:15-16:30 **Flash Communications**

FC13. **Salvador Guardiola**, Target-based de novo design of heterochiral cyclic peptides against the PD-1/PD-L1 interaction

FC14. **Guillermo Bañuelos** Sánchez, Specific Reverse Transcriptase Inhibitors for Mammalian LINE-1 Retrotransposons

FC15. **Raik Artschwager**, Towards the chemo-enzymatic synthesis of a N-glycomimetic library for the targeting of human DC-SIGN



February 19-21, 2020

V GEQB ChemBio Group Meeting

16:30-17:00

COFFEE BREAK + POSTER SESSION 2

17:00-18:30

SESSION 7

Chair: Ana Conejo

17:00-17:45 Oral Communications

OC10. Dynamic stereoselection of kinetically-inert DNA-binding metallopeptide cylinders

Miguel Vázquez-López, CIQUS, Santiago de Compostela, Spain

OC11. GaudiMM: Opening New Horizons in Molecular Modeling of Chemo-biological Systems

Jean-Didier Maréchal, UAB, Barcelona, Spain

OC12. Quinolimide-based probes: New tools to study protein-protein interactions

Juan Antonio González-Vera, University of Granada, Spain

17:45-18:30 Plenary Lecture

Size matters! Controlling the cellular microenvironment yields new insight into the inner working of cells

Wilhelm T. S. Huck, Radboud University, The Netherlands

20:30

CONFERENCE DINNER



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FRIDAY, February 21st, 2020

09:00-11:00

SESSION 8

Chair: Sonsoles Martín Santamaría

09:00-9:45 Plenary Lecture

Breaking the limits in understanding glycan recognition by NMR
Jesús Jiménez-Barbero, Cicbiogune, Bilbao, Spain

09:45-10:15 Invited Lecture

The design of mGlu2 NAMs for neuropsychiatric disorders and studies towards potential tracers for PET imaging
Michiel Van Gool, Janssen, Toledo, Spain

10:15-10:45 Invited Lecture

Conformational landscapes in enzyme design
Silvia Osuna, Universitat di Girona, Spain

10:45-11:05 Flash Communications

FC16. Lucía Tapia, Efficient tyrosine trapping by the supramolecular protection from Src phosphorylation

FC17. Mantas Liutkus, Modular Artificial Light Harvesting Systems

11:05-11:30

COFFEE BREAK + POSTER SESSION 2

11:30-13:30

SESSION 9

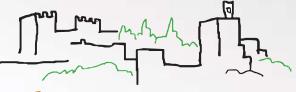
Chair: Eugenio Vázquez

11:30-12:30 Oral Communications

OC13. Non-coding RNAs delivered by Magnetic and Gold Nanoparticles for the treatment of Uveal Melanoma
Álvaro Somoza, IMDEA, Madrid, Spain

OC14. G-quadruplex DNA Structures as Drug Targets for Small Molecules
Jorge González García, University of Valencia, Spain

OC15. Studying the Reaction Mechanism of Orotate Phosphoribosyltransferase by means of X-ray Crystallography and Computational Simulations
Maite Roca, Universitat Jaume I, Castellón, Spain



February 19-21, 2020

V GEQB ChemBio Group Meeting

OC16. (Best PhD thesis GEQB Award)

To be announced

12:30-13:00 **Invited Lecture**

Bioorthogonal turn-on photosensitizers

Olalla Vázquez, Philipps-Universität Marburg, Germany

13:00-13:30 **Invited Lecture**

NMR and biosynthetic gene cluster analysis strategies for the determination of the structure and full absolute configuration of complex microbial natural products

Fernando Reyes, Fundación Medina, Granada, Spain

13:30-13:45 **CLOSING REMARKS & BEST GEQB FLASH & POSTER AWARDS**

13:45-15:00 **MINI-LUNCH**

OC13

sp²-Iminosugar glycolipid mimetics as immunoregulatory agents

E. M. Sánchez-Fernández,¹ M. I. García-Moreno,¹ A. I. Arroba,² M. Aguilar-Diosdado,² J. M. Padrón,³ R. García-Hernández,⁴ F. Gamarro,⁴ J. M. García Fernández,⁵ J.-E. Sánchez-Aparicio,⁶ L. Masgrau,⁶ C. Ortiz Mellet¹

¹University of Seville, Seville, Spain; ²University Hospital of Puerta del Mar, Cadiz, Spain; ³Universidad de La Laguna, Spain; ⁴Instituto de Parasitología y Biomedicina “López Neyra”, Granada, Spain; ⁵Instituto de Investigaciones Químicas, CSIC – University of Seville, Seville, Spain; ⁶Universitat Autònoma de Barcelona, Bellaterra, Spain
esanchez4@us.es

Monosaccharide analogs of the sp²-minosugar family offer unprecedented opportunities to access enzymatically and chemically stable glycoconjugate mimetics amenable to drug discovery programs. In this context, the 1-dodecylsulfonyl-5N,6O-oxomethylidenenojirimycin (DSO₂-ONJ) (Figure 1), a sp²-imino glycolipid (IGL) representative, has shown outstanding anti-inflammatory activity in microglia, reducing gliosis in diabetic db/db mice.¹ DSO₂-ONJ further inhibited the activation of human monocyte-derived dendritic cells (DCs) by lipopolysaccharide (LPS) in vitro and in vivo in a mouse model of acute inflammation.² Biochemical studies and computational docking experiments endorsed a mechanism of action that implies attachment to the allosteric lipid binding pocket of p38α mitogen-activated protein kinase (MAPK), a key protein in the regulation of the innate immune response. This binding mode has also been demonstrated with sp²-IGLs incorporating at the pseudoanomeric position different polyfluoroalkyl segments of varied lengths that facilitate passage through cell membranes. This modification resulted in a 10-fold higher effectiveness at eliciting p38 (Figure 1).³ In this communication we will present the synthesis of different fluorinated sp²-IGLs and their biological evaluation in the context of three pathologies that share common signaling pathways: cancer, Leishmania infection and inflammation.

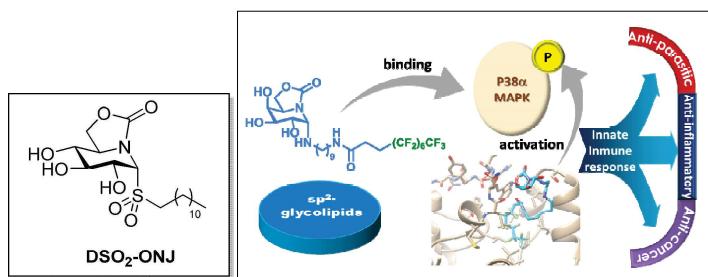


Figure 1. DSO₂-ONJ and polyfluoroalkylsp²-iminosugar glycolipids as immunomodulatory agents.

Acknowledgements

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2. E. Schaeffer, E. M. Sánchez-Fernández, R. Gonçalves-Pereira, V. Flacher, D. Lamont, M. Duval, J.-D. Fauny, J. M. García Fernández, C.G. Mueller, C. Ortiz Mellet, sp²-Iminosugar glycolipids as inhibitors of lipopolysaccharide-mediated human dendritic cell activation in vitro and of acute inflammation in mice in vivo, *Eur. J. Med. Chem.*, **2019**, 169, 111-120.
3. E.M. Sánchez-Fernández, M. García-Moreno, A.I. Arroba, M. Aguilar-Diosdado, J.M. Padrón, R. García-Hernández, F. Gamarro, S. Fustero, J.E. Sánchez-Aparicio, L. Masgrau, J.M. García Fernández, C. Ortiz Mellet, Synthesis of polyfluoroalkylsp²-imino sugar glycolipids and evaluation of their immunomodulatory properties towards anti-tumor, anti-leishmanial and anti-inflammatory therapies, *Eur. J. Med. Chem.*, **2019**, 182, 111604.