



# V GEQB ChemBio Group Meeting

Granada, IPBLN-CSIC Auditorium  
February 19-21, 2020

## PROGRAMME

### WEDNESDAY, February 19th, 2020

- 9:00-10:45 Registration + Coffee
- 10:45-11:00 **GEQB – OPENING**
- Mario Delgado**, IPBLN-CSIC, Granada, Spain  
**Juan Carlos Morales**, IPBLN-CSIC, Granada, Spain
- 11:00-13:30 **SESSION 1**  
Chair: Juan Carlos Morales
- 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. Mulard**, 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**  
Quadruplexes are everywhere, but where exactly?  
**Jean Louis Mergny**, University of Bordeaux, France
- 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
- 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: Francisco Corzana

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. **Ainhoa Oliden Sánchez**, Manipulating ICT in BODIPYs: towards the development of new photosensitizers

FC6. **María Pia Lenza**, Deciphering the N-glycan profile and interactions of FcεR1α by NMR

16:30-17:00

Coffee break + Poster session

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

**THURSDAY, February 20th, 2020**

9:00-11:00 **SESSION 4**

Chair: José Luis Mascareñas

9:00-9:45

**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

9:45-10:15

**Invited Lecture**

Turning stem cells into a medicine

**Mario Delgado**, IPBLN-CSIC, Granada, Spain

10:15-10:45

**Invited Lecture**

Synthetic genetics: beyond DNA and RNA

**Phillip Holliguer**, University of Cambridge, UK

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. **Antonio Delgado-González**, Applying dynamic chemistry for miR-21 direct detection and quantification

11:00-11:30 Coffee break + Poster session

11:30-13:30 **SESSION 5**

Chair: Maria 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

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**, IIQ-CSIC, Seville, Spain

OC6. Visible-light Photoresponsive Ligands for G-quadruplex DNA

**Javier Ramos-Soriano**, University of Bristol, UK

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

16:30-17:00 Coffee break + Poster session

17:00-18:30 **SESSION 7**

Chair: Ana Conejo

17:00-17:45

**Oral Communications**

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

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

OC11. GaudiMM: Opening New Horizons in Molecular Modeling of Chemobiological 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*

**FRIDAY, February 21st, 2020**

9:00-11:00

**SESSION 8**

Chair: Sonsoles Martín Santamaria

9:00-9:45

**Plenary Lecture**

Breaking the limits in understanding glycan recognition by NMR

**Jesús Jiménez-Barbero**, Cicbiogune, Bilbao, Spain

9:45-10:15

**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

FC18. **José Antonio Laz-Ruiz**, Design and development of novel nanodevices for biomedical applications

FC19. **Esther Jiménez Moreno**, Acetals as acid-sensitive cleavable linkers for the design of antibody-drug conjugates

11:05-11:30

Coffee break + Poster session

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

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