

# GRANADA



February 19-21, 2020

## V GEQB ChemBio Group Meeting

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RSEQ  
Real Sociedad Española de Química

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**GRANADA**  
IPBLN-CSIC Auditoriu

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. 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**

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



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### 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 Glyco-dendrimers as Dengue Virus Antagonists  
**María José Hernáiz Gómez**, Universidad Complutense, Madrid, Spain

#### 16:00-16:15 Oral Communication

**OC3.** sp<sup>2</sup>-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

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



Sociedad Española de  
Química Terapéutica

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

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 metallo-peptide 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 Santamaria

09:00-9:45 **Plenary Lecture**

Breaking the limits in understanding glycan recognition by NMR

**Jesús Jiménez-Barbero**, Cibiogune, 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 de 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



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**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**

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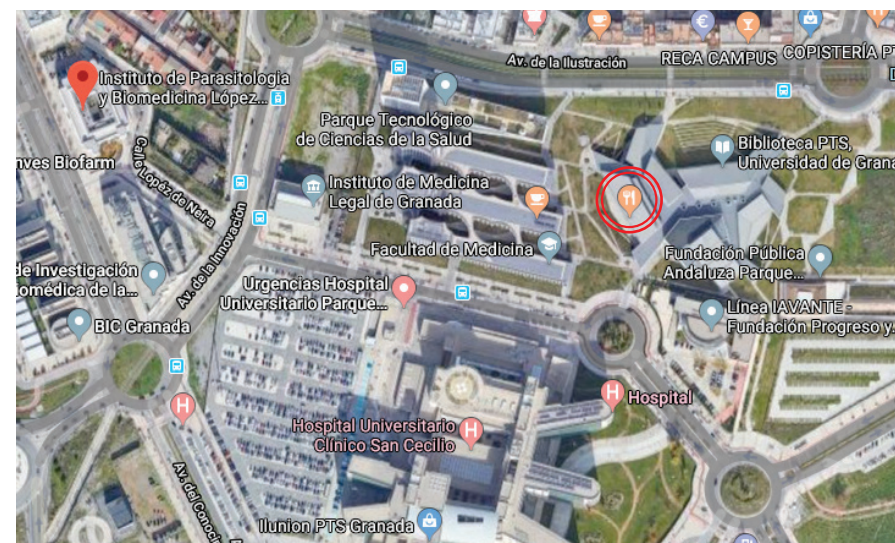


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## Granada Metro Map



## Venue Map





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CONGRESOS

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