

6th

ECBS/LS
EuChemS

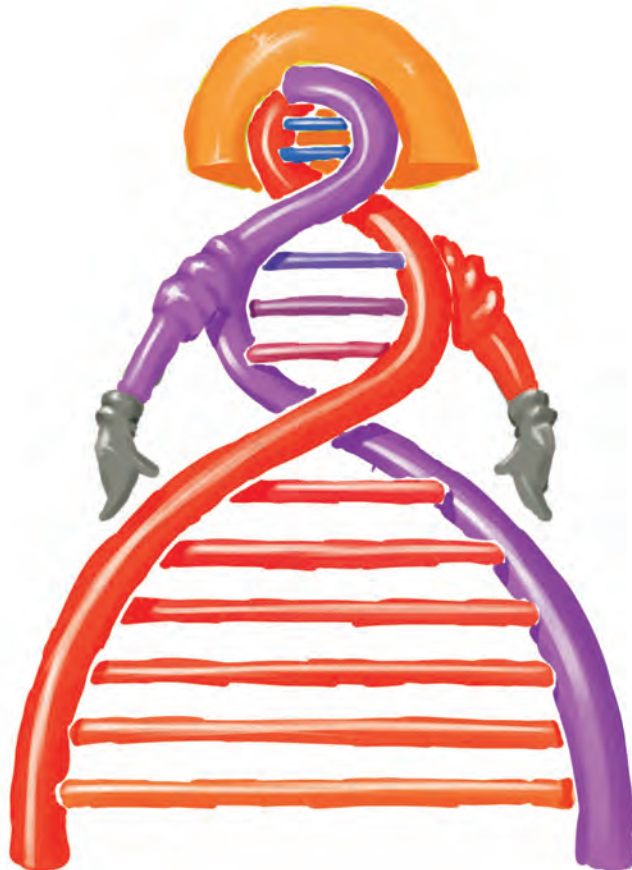
EUROPEAN
CHEMICAL
BIOLOGY
SYMPOSIUM

www.ecbs2019euchems.eu

3-5 APRIL

2019

MADRID-SPAIN



ORGANIZED BY:

 **EuChemS**
European Chemical Society

 **RSEQ**
Real Sociedad Española de Química

eu  openscreen

Presentation

On behalf of the Scientific and Organizing Committees, it is our pleasure to welcome you to Madrid for the **6th ECBS/LS-EuChemS** meeting. This occasion brings together the **6th European Chemical Biology Symposium** and the meeting of the **EuChemS Division "Chemistry in Life Sciences" (LS-EuChemS)** and it is jointly organized by EuChemS and EU-OPENSREEN. This meeting builds on the success of 4th ICBS/ECBS joint meeting in Berlin (2015) and 5th ECBS in Budapest (2017).

Chemical biologists from all parts of Europe and overseas come together to present and discuss the latest achievements in cutting edge chemical sciences. This present joint meeting gathers researchers from organic & biological chemistry, proteins biotechnology, computational biology, protocells, machine learning, bacterial resistance, drug discovery, synthetic biology, biomedical materials and chemical glycobiology.

A number of young researchers will present their work at the meeting (oral & flash presentations were selected from abstracts), discuss with the speakers and embrace the exciting developments currently happening in chemical biology.

The venue for the **6th ECBS/LS-EuChemS** meeting will be at CSIC headquarters beautifully located near to Madrid city center. It offers a perfect base for exploring the historic centre of Madrid.

We are looking forward to meeting you in Madrid!

Dr. Sonsoles Martín-Santamaría

EuCheMS Division of "Chemistry in Life Sciences Division", Chair

Dr. Philip Gribbon

EU-OPENSREEN Coordinator

Organizing Committee

Sonsoles Martín-Santamaría (Chair)

Center for Biological Research, CIB-CSIC, Spain

Philip Gribbon (Chair)

EU-OPENSCREEN, Deutschland

Bahne Stechmann

EU-OPENSCREEN, Deutschland

Jordi Quintana

University Pompeu Fabra, Spain

Katja Herzog

EU-OPENSCREEN, Deutschland

Joan Guzmán-Caldentey

Center for Biological Research, CIB-CSIC, Spain

Valle Palomo

Center for Biological Research, CIB-CSIC, Spain

Elena Gómez-Rubio

Center for Biological Research, CIB-CSIC, Spain

Scientific Committee

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Center for Biological Research, CIB-CSIC, Spain

Philip Gribbon (Chair)

EU-OPENSCREEN, Deutschland

José Luis Mascareñas

CIQUS, University of Santiago de Compostela, Spain

Bahne Stechmann

EU-OPENSCREEN, Deutschland

Jordi Quintana

University Pompeu Fabra, Spain

Marko D. Mihovilovic

Vienna University of Technology, Austria

María Jesús Vicent

CIPF, Spain

Krister Wennerberg

FIMM-EMBL, FI

Petr Bartunek

Institute of Molecular Genetics, Czech Republic

Alleyn Plowright

Sanofi, Deutschland (EFMC representative)

Haian Fu

Emory University, USA (ICBS representative)

Programme

Wednesday, 3rd April

- 09:30 Registration
- 10:50 OPENING
Elena Domínguez – CSIC Vice-President
Enrique de la Rosa – CIB-CSIC Director
Wolfgang Fecke – Director General EU-Openscreen
Sonsoles Martín-Santamaría – Chair
Philip Gribbon – Chair
- 11:00 **SESSION I. ICBS Session**
Chair: Haian Fu
PLENARY LECTURE
Synthetic Protobiology
Stephen Mann – University of Bristol, UK
- 11:45 INVITED LECTURE
Illuminating the Biochemical Activity Architecture of the Cell
Jin Zhang – UCSD, USA
- 12:15 ORAL COMMUNICATIONS
OC1: Jacek Kolanowski – IBCH-PAS, PL
Fluorescent probes for multiparametric investigation of biochemical analytes in cellular models
OC2: Salvador Tomás – Birbeck-University of London, UK
Protocells promote complexity within: self-assembly and condensation

- 12:45 **Lunch break & Poster Session**
- 14:00 **SESSION II**
Chair: Francesco Peri
PLENARY LECTURE
Lectins from Bacteria and Fungi: Therapeutical Targets and Research Tools
Anne Imberty – CNRS, FR
- 14:45 **ORAL COMMUNICATIONS**
OC3: Antoni Planas – IQS, ES
Dual N-acetylglucosamine and N-acetylmuramic peptidoglycan deacetylation. Specificity and biological functions
OC4: Derek S. Tan – Memorial Sloan Kettering Cancer Center, USA
Diversity and design: new chemical probes for biology and medicine
- 15:15 **FLASH COMMUNICATIONS**
FC1: Benedikt Heinrich – University of Marburg, ES
Far-red fluorescent DNA binder allows host-pathogen interaction studies of multidrug-resistant bacteria

FC2: Diana Rodríguez – *CIQUS-USC, ES*

Novel covalent inhibitors of carbapenem-hydrolyzing class D β -lactamases enzymes for disabling antibiotic resistance in superbugs

FC3: Alba Vázquez Arias – *University of Vigo, ES*

Exploring bacterial surface display as a platform for developing engineered glycan-binding proteins

15:30 INVITED LECTURE

Effects of Antibiotics on Cell Cycle Progression of Staphylococcus aureus

Mariana Gomes de Pinho – *ITQB, PT*

16:00 **Coffee break & Poster Session**

16:30 **SESSION III. EU Openscreen ERIC Session**

Chair: Jordi Quintana

INVITED LECTURE

Applying Established Concepts of Pharmaceutical Development to Industrialization of Cellular Cancer Immunotherapy

Margit Jeschke – *Novartis, CH*

17:00 ORAL COMMUNICATIONS

OC5: Bahne Stechmann – *EU-OPENSREEN, DE*

Access models for eu-openscreen eric

OC6: Albert A. Antolin – *ICR, UK*

Probe miner v2: updated objective data-driven assessment of chemical probes

17:30

ORAL COMMUNICATIONS

OC7: Marie Louise Jung – *Prestwick Chemical, FR*
Smart screening libraries over the past 20 years and success stories in medicinal chemistry

OC8: Bernhard Ellinger – *Fraunhofer IME, DE*
Validation of a high content assay to identify DNAJB6 agonists

OC9: Francisca Vicente – *MEDINA, ES*

A novel natural product for pancreatic cancer

18:15

FLASH COMMUNICATIONS

FC4: José García-Tenorio – *Molport, LV*

Screening compounds & building blocks sourcing and procurement solution in a customized way

FC5: M^a Angélica Luque-González – *GENYO-UGR, ES*

Trypanosomatids identification by chem-NAT technology

FC6: Bruno Cuevas Zuviría – *CBGP-UPM, ES*

aAMDlib: testing transferability of electron density models on chemical libraries with biological interest

20:15

Speakers & Committees dinner

Thursday, 4th April

08:30

SESSION IV. RSEQ-GEQB Session

Chair: Concepción González-Bello

PLENARY LECTURE

DNA Simulations from the Electron to the Chromosome... and Beyond

Modesto Orozco – *IRB Barcelona, ES*

09:15

ORAL COMMUNICATIONS

OC10: Gonzalo Jiménez Osés – *University of La Rioja, ES*

Computer design and directed evolution of a highly active and enantioselective metallo-hetero-diels-alderase

OC11: Macarena Sánchez Navarro – *IRB Barcelona, ES*

Paving the way towards the brain delivery of biotherapeutics: Modification of proteins with blood-brain barrier peptide shuttles

09:45

INVITED LECTURE

What Do We Know about Ion Conduction in Ion Channels?

Carmen Domene – *University of Bath, UK*

10:15

FLASH COMMUNICATIONS

FC7: Ángela Rodríguez-Costa – *CIQUS-UCS, ES*

Hydroxylamine derivatives for specific lysine covalent modification of bacterial type I dehydroquinase

FC8: Andrea Canal Martín – *CIB-CSIC, ES*

Thiol-disulfide reversible chemistry in non-conventional conditions

FC9: Nuria Lafuente-Gómez – *IMDEA nanoscience, ES*

Functionalization of magnetic nanoparticles with gemcitabine via disulfide bonds: a new approach for the pancreatic cancer treatment

10:30

Coffee Break & Poster Session

11:00

SESSION V

Chair: Philip Gribbon

INVITED LECTURE

Combining Cheminformatics and Bioinformatics in Drug Discovery - Lessons Learned and New Opportunities

Gerard JP van Westen – *University of Leiden, NL*

11:30

ORAL COMMUNICATIONS

OC12: María Duca – CNRS, FR

Synthetic small-molecule RNA ligands: scope and applications

OC13: Olalla Vazquez – Philipps / Universität Marburg, DE

Optochemical Tools for Biological Processes

12:00

ORAL COMMUNICATIONS

OC14: José Brea – UCS - Innopharma, ES

Therapeutic potential of blood glutamate grabbing in stroke: a proof of concept

OC15: David Albesa-Jové – CIC bioGUNE, ES

Deciphering the mechanism of action of toxins delivered by the type-VI secretion system (t6ss) in *pseudomonas aeruginosa*

12:30

FLASH COMMUNICATIONS

FC10: Ferrán Feixas – IQCC, ES

Accelerating (bio)molecular recognition and assembly

FC11: Davide Avagliano – ITC, AT

Drastic effect of the electrostatic energy on the binding mode of spiropyran photoprobe to dsDNA

FC12: María J. Matos – USC, ES

Neurodegenerative diseases: from small molecules to targeted therapies

12:45

Lunch break & Poster Session

14:00

SESSION VI

Chair: María J. Vicent

PLENARY LECTURE

Multiplexing and Multivalency in Nanomedicine Design

Giuseppe Battaglia – University College of London, UK

14:45

ORAL COMMUNICATIONS

OC16: Gustavo Bodelón – University of Vigo, ES

Plasmonic ZIF8 metal-organic frameworks (MOFs) with self-assembled proteins as optical probes for imaging cell surface receptors

OC17: Luca Laraia – Technical University of Denmark, DK

New tool compounds for studying autophagy

15:15

FLASH COMMUNICATIONS

FC13: Carlota Tosat – CIB-CSIC, ES

Specific Biosensors in Drug Discovery for Amyotrophic Lateral Sclerosis

FC14: Marisa Juanes – CIQUS-UCS, ES

Amphiphilic peptide/Cas9 nanocomplexes for the delivery of gene editing nucleases

FC15: Andreia Mónico – CIB-CSIC, ES

Computational modeling and cysteine crosslinking studies of vimentin

15:30

INVITED LECTURE

New Peptides Designs for Gene Delivery, Genetic Edition and the Preparation of Cytoskeleton Mimics

Javier Montenegro – *CIQS-USC, ES*

16:00

Coffee Break & Poster Session

16:30

SESSION VII

Chair: Juan Carlos Morales

INVITED LECTURE

Merging Magnetic Hyperthermia with other Anticancer Treatments for Tackling Cancer

Teresa Pellegrino – *IIT, IT*

17:00

ORAL COMMUNICATIONS

OC18: Amadeu Llebaria – *IQAC-CSIC, ES*

Precise control of GPCR receptors with light and allosteric photoswitchable ligands in cells and living animals

OC19: Luís Pinto da Silva – *CIQUP, PT*

Preparation and Evaluation of Self-Illuminating Photosensitizers for Photodynamic Therapy of Cancer

17:30

INVITED LECTURE

Perturbation of mitochondrial genome stability with OGG1 inhibitors as a novel strategy to treat cancer

Torkild Visnes – *SINTEF Industry/ Karolinska Institutet, NO*

18:00

FLASH COMMUNICATIONS

FC16: Paula Milán Rois – *IMDEA nanoscience, ES*
Reprogramming Uveal Melanoma Cells: A Combination Therapy Based on Gold Nanoparticles

FC17: Antonio Aires – *CIC biomaGUNE, ES*
Green synthesis of designed protein-stabilized CdS quantum dots for bio-imaging applications

FC18: Carmen Yuste-Calvo – *GBGP-UPM-INIA, ES*
Functionalization of elongated viral nanoparticles through chemical conjugation to molecules of different kinds

FC19: Giulia Caron – *University of Torino, IT*
Ro5 vs bRo5: the winner is ...

FC20: Marta Sanz-Murillo – *CIB-CSIC, ES*
Structural basis of RNA polymerase I stalling at UV light-induced DNA damage

FC21: Fabio Alessandro Facchini – *Università degli studi di Milano-Bicocca, IT*
FP7, a synthetic TLR4 antagonist, reduces inflammation in the Gastrointestinal Tract

20:30

Conference Dinner

Friday, 5th April

08:30

SESSION VIII. RSEQ Session

Chair: Itziar Alkorta

PLENARY LECTURE

Beyond Watson and Crick: Chemical Modifications in G-Quadruplexes Regulate Gene Expression

Cynthia J. Burrows – *University of Utah, USA*

09:15

ORAL COMMUNICATION

OC20: Ruth Pérez Fernández – *CIB-CSIC, ES*

Protein-directed Dynamic Systems: Insights into Real Time Chemical Processes

09:30

FLASH COMMUNICATIONS

FC22: Iris Alicia Bermejo – *University of La Rioja, ES*

Insights into the molecular recognition and conformational preferences of the STn antigen derived glycopeptides as tools in cancer vaccination and diagnosis

FC23: Beatriz Fernández de Toro – *CIB-CSIC, ES*

Resolving extended N-glycans by NMR: New insights into influenza hemagglutinin N-glycan interactions

FC24: Ana Díaz-Fernández – *University of Oviedo, ES*

Selection of aptamers recognizing the glycosylation site of PSA: aptasensors for detection of cancer-related glycosylation changes

09:45

INVITED LECTURE

Artificial Metalloenzymes: Challenges and Opportunities

Thomas R. Ward – *University of Basel, CH*

10:15

ORAL COMMUNICATION

OC21: Marc García-Borrás – *IQCC, ES*

Computational characterization of enzymatic reactive intermediates for the discovery and design of new biocatalytic activities

10:30

Coffee break & Poster Session

11:00

SESSION IX. EFMC Session

Chair: Yves P. Auberson (EFMC President)

INVITED LECTURE *Sponsored by ChemPubSoc Europe*

Discovery and Development of Antibiotics from (Myxo)bacterial Secondary Metabolites

Rolf Müller – *Helmholtz-HZI, DE*

11:30

ORAL COMMUNICATIONS

OC22: Mariapina D'Onofrio – *University of Verona, IT*

Introduction of post-translational modifications in vitro modulates TAU protein fibrillation

OC23: Manfred Jung – *University of Freiburg, DE*

Targeted release of epigenetic histone demethylase inhibitors via enzymatic bioreductive activation from prodrugs

12:00 INVITED LECTURE
Repurposing Ciclopirox as a Pharmacological Chaperone

Oscar Millet – *CIC bioGUNE/ATLAS, ES*

12:30 ORAL COMMUNICATION

OC24: M. Eugenio Vázquez – *University of Santiago, ES*

Dynamic stereoselection of kinetically-inert DNA-binding metallopeptide cylinders

12:45 **Lunch break & Poster Session**

14:00 **SESSION X. EuChemS Session**

Chair: Sonsoles Martín-Santamaría

INVITED LECTURE

Mechanistic insights into the Function of HSP90 Co-chaperones by cryo-EM

Oscar Llorca – *CNIO, ES*

14:30 ORAL COMMUNICATION

OC25: Marc Nazare – *FMP, DE*

Selective Tankyrase Inhibitors Through a Structure-guided Deconstruction and Hybridization Approach

14:45 INVITED LECTURE
Stabilization of 14-3-3 Protein-Protein Interactions

Christian Ottman – *Eindhoven University of Technology, NL*

15:15 CLOSING PLENARY LECTURE (IYPT)
The Biological Chemistry of Selected Elements from the Periodic Table

Federico Gago – *University of Alcalá, ES*

16:00 CLOSING, AWARDS & FINAL REMARKS
Best Poster and Flash Communications awards. PhD Tesis 2018 Award of the RSEQ Chemical Biology Division to Dr. Elsa Hernando.

Pilar Goya – *EuChemS President*

Sonsoles Martín-Santamaría – *Chair*

Philip Gribbon – *Chair*

Venue

The congress venue is the historic headquarters **Main Building of the Spanish National Research Council, CSIC** (Consejo Superior de Investigaciones Científicas) in Madrid, placed in the **CSIC campus of 117 Serrano street**. The place is very well communicated by public transport, either subway (República Argentina station of line 6 of Metro) or bus (various bus lines stop in Serrano street, very near the CSIC campus).



CSIC Building Serrano Street, 117. 28006 Madrid. Spain



Lunches, coffee breaks and conference dinner

Coffee Breaks and some lunches will be offered at the hall of the CSIC main building.

Some lunches will be offered at the CSIC Residence located in an annex building. Please, check lunch tickets and map for location.

Conference dinner will be served at the Palacio de Cibeles located in Plaza de Cibeles, 1. Dinner is not included in the registration fee. The price is 40 €.



(*) Access to Metro Sevilla (500 m)

Registration

Technical Secretariat will offer the following opening times:

- Wednesday, April 3rd: 09:30 – 19:00
- Thursday, April 4th: 08:30 – 19:00
- Friday, April 5th: 08:30 – 16:30

Internet access

There is available a wifi network during the congress days:

SSID: ECBS

Password: Abril2019

Technical Secretariat

Fundación General de la Universidad de Alcalá
Dpto. de Formación y Congresos

C/ Imagen 1 y 3

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Notes

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