



PROGRAMME

WEDNESDAY, 3 APRIL

- 09:30 **Registration**
- 10:50 **OPENING**
Elena Domínguez - CSIC Vice-President
María Jesús Fernández Martínez- CIB-CSIC Director
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

20:30 **Speakers & Committees dinner**

THURSDAY, 4 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 – CIQUES-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 - CIQUS-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

SE 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

FP7, a synthetic TLR4 antagonist, reduces inflammation in the Gastrointestinal Tract



20:30 Conference Dinner

FRIDAY, 5 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 del 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) and **Philip Gribbon** (Chair).