

X National Conference BIFI21.

Scientific Program.

February 3rd

09:30-09:45 **Opening Ceremony (BIFI Director)**

Biochemistry and MCB / Chair: Jesús Clemente-Gallardo

Gene regulation and physiology of cyanobacteria.

09:45-10:15 **Maria F. Fillat**, FUR proteins from *Anabaena* sp. PCC7120: beyond the control of metal Homeostasis. Ref. 01PI.

10:15-10:30 **Jorge Guío**, Lin genes in *Anabaena* sp. PCC7120: experimental bases for the development of a lindane biosensor. Ref. 01T.

Apoptosis and Metabolism.

10:30-11:00 **José A. Carrodegua**s, Cellular models to investigate Parkinson's alpha-synuclein aggregation and cell-to-cell transmission. Ref. 02PI.

11:00-11:15 **Diego de la Fuente**, Crosstalk between alpha-synuclein and ubiquitin in Parkinson's disease. Ref. 02T.

11:15-11:45 Break

Physics and Computation / Chair: Jesús Clemente-Gallardo.

Physical modelling of biomolecules.

11:45-12:15 **Alessandro Fiasconaro**, Overview and updates on the Physical Modelling of Biomolecules research line. Ref. 03PI.

12:15-12:45 **Antonio Rey**, Simulation of protein folding in confined and/or crowded environments. Ref. 04PI.

12:45-13:00 **David Luna**, Some strategies to test and refine a statistical inference model for antibody sequences. Ref. 03T.

Theoretical and applied modeling of complex systems

13:00-13:30 **Jesús Gómez-Gardeñes**, Modeling and analysis of COVID-19 diffusion by integrating multiple interactions and mobility patterns. Ref. 05PI.

13:30 - 13:45 **Sergio Faci**, A framework for joint explosive percolation and synchronization Transitions. Ref. 04T.

13:45 - 14:00 **Adriana Reyna**, Virus spread versus contact tracing: Two competing contagion processes. Ref. 05T.

14:00-15:30 Lunch Break.

Biophysics / Chair: Nunilo Cremades

Protein folding & Molecular design.

15:30 - 16:00 **Javier Sancho**, Proteins as molecules to understand and modulate. Ref. 06PI.

16:00 - 16:15 **Juan José Galano Frutos**, PirePred: linking Bioinformatics to clinical diagnosis. Ref. 06T.

16:15 - 16:30 **Helena García Cebollada**, Computational pathogenicity prediction in Rett Syndrome using 2DRMSD clustering. Ref. 07T.

Signal transduction & membrane protein therapies

16:30 - 17:00 **Javier García-Nafría**, Signal transduction & membrane protein therapies. Ref. 07PI.

Structural biology of brain receptor complexes

17:00 - 17:15 **Beatriz Herguedas**, Structural biology of brain receptor complexes. Ref. 08PI.

17:15-18:30 Poster Session 1.

Ref. P01 **Teresa Bes**, Exploring FurA interaction with photosynthetic electron carrier proteins in *Anabaena* sp. PCC7120.

Ref. P02 **Sergio Boneta**, Computational insights on the hydride transference of the human Apoptosis Inducing Factor (hAIF) enzyme.

Ref. P03 **José D. Camino**, Towards a physiologically relevant aggregation pathway of α -synuclein in Parkinson's disease.

Ref. P04 **Javier Casado**, The ArsR response regulator: a novel and validated therapeutic target against *Helicobacter pylori* infection.

Ref. P05 **Pablo Gracia**, Dual Color Time-Resolved Fluorescence Spectroscopy: a Framework for Studying Small Molecule-Amyloid Interactions.

Ref. P06 **Jorge Guío**, Identification of regulatory networks performed by the Ferric Uptake Regulator FurA in *Anabaena* sp. PCC7120.

Ref. P07 **Marta Martínez-Júlvez**, Biochemical characterisation of MurA: an essential component in peptidoglycan cell wall biosynthesis.

Ref. P08 **Francho Nerín**, Expanding a Molecular Dynamics-based method for the calculation of protein stability from first principles.

Ref. P09 **Asier Urriolabeitia**, Rh-NHC catalyzed head-to-tail alkyne dimerization enhanced by metal-ligand cooperation.

18:30 **BIFI Council Meeting**

February 4th

Physics and Computation / Chair: Joaquín Sanz

Spin glasses.

9:30 - 10:00 **Javier Moreno-Gordo**, Temperature chaos is present in off-equilibrium spin-glass dynamics. Ref. 09PI.

Molecular structure and electronic dynamics

10:00 - 10:15 **Carlos Bouthelier**, Entropy and canonical ensemble of hybrid quantum classical systems. Ref. 08T.

Computation Science

10:15 - 10:45 **Daniel Martínez**, Systems, Support and Supercomputing. Ref. 10PI.

Citizen Science

10:45 - 11:15 **Jesús Clemente-Gallardo**. Citizen Science in Zaragoza: recent collaborations of BIFI and Ibercivis Foundation. Ref. 11PI.

11:15-11:45 Break

Biophysics / Chair: Javier García Nafría.

Biomolecular interactions.

11:45 - 12:30 **Adrián Velázquez-Campoy**, Biomolecular interactions, drug discovery, LACRIMA and ZCAM. Ref. 12PI.

12:30 - 12:45 **David Ortega-Alarcón**, Translational research in MeCP2-related diseases. Ref. 09T.

Flavoenzymes: action mechanisms & Biotechnology

12:45 - 13:15 **Milagros Medina**, Flavoenzymes as versatile catalysts: gaining basic knowledge to develop Biotech and Biomed tools. Ref. 13PI.

13:15 - 13:30 **Nerea Novo**, W483 in the apoptosis inducing factor: thermodynamic, kinetic and dynamic implications for NADH oxidation. Ref. 10T.

13:30 - 13:45 **Martha Minjarez-Sáenz**, The flavoproteome of *Brucella ovis* in the search of antimicrobial targets: MurB, a promising candidate. Ref. 11T.

13:45-15:15 Lunch Break.

Biophysics / Chair: Nunilo Cremades.

Clinical Diagnosis and Drug Delivery.

15:15 - 15:45 **Olga Abián**, Clinical Diagnosis and Drug Delivery. Ref. 14Pl.

15:45 - 16:00 **Ana Jiménez-Alesanco**, Drug discovery for inhibiting 3CLPro: an essential protease of SARSCoV-2. Ref. 12T.

Biochemistry and MCB / Chair: Nunilo Cremades.

***Mycobacterium tuberculosis*.**

16:00 - 16:30 **Jesús Gonzalo Asensio**, Some reasons to study the adaptation of *Mycobacterium tuberculosis* to its human host. Ref. 15Pl.

16:30 - 16:45 **Juan Calvet Seral**, *Mycobacterium tuberculosis* PhoP-reporter strains for testing potential anti-virulence molecules. Ref. 13T.

Development of antimicrobials and mechanisms of resistance

16:45 - 17:15 **José A. Aínsa**, Antimicrobial “magic bullets” in the 21st century. Ref. 16Pl.

17:15 - 17:30 **José Manuel Ezquerro**, Strategies to elucidate the mode of action of avermectins against mycobacteria. Ref. 14T.

17:30-19:00 Poster Session 2.

Ref. P10 **Martha Minjárez-Sáenz**, The flavoproteome of *Brucella ovis* in the search of antimicrobial targets: MurB, a promising candidate.

Ref. P11 **Violeta Morcuende**, A novel approach for early cancer detection based on dendrimer nanoparticles.

Ref. P12 **Irene Oliván**, Unraveling biofilm formation in the filamentous cyanobacterium *Anabaena* sp. PCC7120.

Ref. P13 **Cristina Sarasa-Buisán**, Expanding the FurC regulon from *Anabaena* sp. PCC7120: *in silico* approach and experimental validation of novel FurC targets.

Ref. P14 **David Soriano-Paños**, Influence of recurrent mobility patterns on the spread of vector-borne diseases.

Ref. P15 **Ernesto Anoz-Carbonell**, The Catalytic Cycle of Human NQO1: Hydride Transfer, Conformational Dynamics, and Functional Cooperativity.

Ref. P16 **Sonia Hermoso-Durán**, Thermal Liquid Biopsy (TLB) applied to Pancreatic Cyst Diagnosis.

Ref. P17 **Nerea Novo**, W483 in the apoptosis inducing factor: thermodynamic, kinetic and dynamic implications for NADH oxidation.

Ref. P18 **David Polanco**, Characterization of the aggregation pathway of Parkinson's related amyloid protein alpha-synuclein under liquid-liquid phase separation.

Ref. P19 **Patricia Bruñén**, Design and synthesis of FMN derivatives for covalent binding to *Anabaena* apoflavodoxin.

February 5th

Physics and Computation / Chair: Joaquín Sanz.

Complex systems & Networks.

09:30 - 10:00 **Yamir Moreno**, Research lines @ COSNET Lab. Ref. 17PI.

10:00 - 10:15 **Carlos Gracia**, Game Theory: Modeling from experimental results. Ref. 15T.

10:15 - 10:30 **Alberto Aletá**, Modeling COVID-19: A Quest for Data. Ref. 16T.

Biophysics / Chair: Joaquín Sanz.

Protein misfolding & amyloid aggregation.

10:30 - 11:00 **Nunilo Cremades**, Pathological protein self-assembly mechanisms and single-molecule experimental tools for their study. Ref. 18PI.

11:00 - 11:15 **Pablo Gracia**, Dual Color Time-Resolved Fluorescence Spectroscopy: a Framework for Studying Small Molecule-Amyloid Interactions. Ref. 17T.

11:15-11:45 Break

Biophysics / Chair: Nunilo Cremades.

Protein glycosylation and its role in disease.

11:45 - 12:15 **Ramón Hurtado**, Why glycosylation matters in health and disease? Ref. 19PI.

12:15 - 12:30 **Ana García-García**, Structural basis for substrate specificity and catalysis of 1,6- fucosyltransferase. Ref. 18T.

Associated Units / Chair: Nunilo Cremades.

12:30 - 13:00 **Inmaculada Yruela** (*Aula Dei-CSIC / Structural and Computational Biology*), The RDI Unit 'GBsC' (BIFI-Unizar) associated to the CSIC: a holistic practice in the investigation of genes and proteins. Ref. 20PI.

13:00 - 13:30 **Juan Hermoso** (*IQF"Rocasolano"-CSIC / Structural Biology and Crystallography*), From Fundamental Processes to Biotechnology and Biomedicine. A Glimpse of Structural Research at CBE-IQFR. Ref. 21PI.

13:30 - 14:00 **Douglas V. Laurents** (*IQF"Rocasolano"-CSIC / Protein NMR group*), Ongoing Research in the "Manuel Rico" NMR Laboratory. Ref. 22PI.

14:00-15:30 Lunch Break

Biochemistry and MCB / Chair: Javier García Nafría.

Functional genomics of the OXPHOS system.

15:30 - 15:45 **Patricio Fernández**, How hot are mitochondria? Ref. 23PI.

15:45 - 16:00 **Raquel Moreno-Loshuertos**, Real-Time Intracellular Temperature Imaging Using Lanthanide-Bearing Nanoparticles. Ref. 24PI.

16:00 - 16:15 **Ruth Soler-Agesta**, Mechanism of dichloroacetate-induced cell death in highly tumorigenic and glycolytic cancer cells. Ref. 19T.

Computational genomics and systems Bio-medicine

16:15 - 16:45 **Joaquín Sanz**, Computational genomics and systems Bio-medicine: a new research line at BIFI. Ref. 25PI.

16:45 - 17:00 **Mario Tovar Calonge**, A Bayesian approach to minimize bias and uncertainty in impact evaluation of tuberculosis vaccines. Ref. 20T.

17:00 - 17:15 **Ignacio Marchante Hueso**, Using single-cell RNA-sequencing to characterize genetic ancestry effects on the response to viral infection. Ref. 21T.

Plant evolutionary biology

17:15 - 17:45 **Pilar Catalán**, Gradual polyploid genome evolution of model Brachypodium grasses revealed by pangenomic analysis. Ref. 26PI.

17:45 - 18:00 **Rubén Sancho**, PhyloSD: Phylogenomic detection of known and ghost subgenomes of polyploid plants. Ref. 22T.

18:00 **Concluding remarks and poster prizes.**