

– XI NATIONAL CONFERENCE PROGRAM –

# ***BIFI 2023***

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**25<sup>th</sup> – 27<sup>th</sup>**

JANUARY

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**ZARAGOZA / SPAIN**



**Universidad  
Zaragoza**

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## Wednesday, January 25th

08:30 - 08:45 **Registration.** (BIFI secretary)

08:45 - 09:00 **Opening ceremony.**

### Session 1. January 25<sup>th</sup>, 09:00-11:00 h. Chair: Milagros Medina

#### Protein misfolding and amyloid aggregation.

09:00 - 09:30 **N. Cremades**, Novel fluorescence-based tools and applications in protein amyloid aggregation: from basic research to diagnosis. Ref. [01PI](#).

09:30 - 09:45 **D. Polanco**, Novel pathways of  $\alpha$ -synuclein aggregation and toxicity through liquid-liquid phase separation. Ref. [01T](#).

09:45 - 10:00 **A. Carrancho**, Development and validation of a novel biomarker-based diagnostic method for Parkinson's disease. Ref. [02T](#).

#### Signal transduction and membrane protein therapies.

10:00 - 10:30 **J. García-Nafría**, Functional mechanisms of G protein-coupled receptors and their therapeutics. Ref. [02PI](#).

#### Structural Biology of neuronal membrane receptors.

10:30 - 11:00 **B. Herguedas**, Ion channel structural biology: from protein production to structure determination. Ref. [03PI](#).

### 11:00-11:30 h. Coffee Break

### Session 2. January 25<sup>th</sup>, 11:30-13:30 h. Chair: Javier García-Nafría

#### Computational Genomics and Systems Bio-Medicine.

11:30 - 12:00 **J. Sanz**, Alveolar macrophages responses to *Mycobacterium tuberculosis* infection: ontogenetic determinants and HIV-coinfection effects. Ref. [04PI](#).

12:00 - 12:15 **I. Marchante**, Uncovering the transcriptomic footprint of inter-individual heterogeneity in Celiac Disease. Ref. [03T](#).

12:15 - 12:30 **J. Bertol**, Multi-omics portrait of VirR protein function in cell wall remodeling and vesiculogenesis in *Mycobacterium tuberculosis*. Ref. [04T](#).

#### External Contribution

12:30 - 12:45 **C. Ortega-Sabater**, Untangling the impact of chromosomal instability in the progression of pediatric B-Acute Lymphoblastic Leukemia with aneuploidies through mathematical models and single-cell analyses. Ref. [05T](#).

#### Statistical-Physics Modeling of biomolecules

12:45 - 13:15 **P. Bruscolini**, Ongoing activity in the "Physical Modeling of Biomolecules" research line. Ref. [05PI](#).

13:15 - 13:30 **A. Sáinz-Agost**, Resonant effects in polymer translocation under transversal fields. Ref. [06T](#).

**13:30-15:30 h. Lunch Break.**

**Session 3. January 25<sup>th</sup>, 15:30-17:00 h. Chair: Pierpaolo Bruscolini**

**Protein glycolylation and its role in disease.**

15:30 - 16:00 **V. Taleb**, Structural and mechanistic insights into the cleavage of clustered O-glycan patches-containing glycoproteins by mucinases of the human gut. [06PI](#).

16:00 - 16:15 **A.M. González-Ramírez**, Structural basis for the synthesis of the core 1 structure by C1GalT1. Ref. [07T](#).

**High performance and cloud computing**

16:15 - 16:45 **D. Martínez / C. Gimeno**, Computing services at BIFI: Past, present and futuro. Ref. [07PI](#).

16:45 - 17:00 **S. Martínez-Losa del Rincón**. Quantum Technologies in the near future: The second Quantum Revolution. Ref. [08T](#).

**17:00-17:30 h. Coffee Break.**

**Poster Session 1. January 25<sup>th</sup>, 17:30-19:30 h.**

## Thursday, January 26<sup>th</sup>

### Session 4. January 26<sup>th</sup>, 09:00-11:00 h. Chair: Jesús Gonzalo-Asensio.

#### Invited speaker.

09:00 - 09:45 **R. Prados-Rosales**, Dynamin-like proteins are required for secretion of extracellular vesicles and virulence of *Mycobacterium tuberculosis*. Ref. [08PI](#).

#### External contribution

09:45 - 10:00 **P. Fernández**, A lipidomic approach to the understanding of Long-COVID. Ref. [09T](#).

#### Flavoenzymes: action mechanisms and biotechnology

10:00 - 10:30 **P. Ferreira**, Human Apoptosis inducing factor: recent answers to some old questions. Ref. [09PI](#).

10:30 - 10:45 **A. Moreno**, Repositioning drugs to inhibit MurA (UDP-N-acetylglucosamine 1-carboxyvinyltransferase UDP-N-acetylglucosamine 1-carboxyvinyltransferase), an enzyme committed to the biosynthesis of peptidoglycan in *Brucella ovis*. Ref. [10T](#).

10:45 - 11:00 **S. Boneta**, The use of QM/MM calculations to study the hydride transference on flavoenzymes. Ref. [11T](#).

### 11:00-11:30 h. Coffee Break

### Session 5. January 26<sup>th</sup>, 11:30-13:30 h. Chair: Carlos Gracia-Lázaro

#### Digital Science.

11:30 - 12:00 **C.P. Llantada**, "Help us better understand our changing climate": Functions of language in Citizen Science communication. Ref. [10PI](#).

12:00 - 12:15 **O.M. Carciu**, Evaluative polarity in a small-scale corpus of significance statements. Ref. [12T](#).

12:15 - 12:30 **R. Villares**, Communicating science on Twitter conference presentations. Ref. [13T](#).

#### Data analysis, advanced visualization and technology transfer

12:30 - 13:00 **G. Ruiz**, EOSC-Synergy: Hackathon Manager, a tool for organising hackathons. Ref. [11PI](#).

#### Molecular dynamics and electronic structure

13:00 - 13:15 **C. Bouthelier-Madre**, Exact Factorization of molecular wave function, Hamiltonian dynamics and its semiclassical limits: a search for consistent hybrid systems. Ref. [14T](#).

13:15 - 13:30 **A. Urriolabeitia**, Mechanistic insight into the selective reduction of CO<sub>2</sub> catalyzed by an Ir complex and B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>. Ref. [15T](#).

### 13:30-15:30 h. Lunch Break.

**Session 6. January 26<sup>th</sup>, 15:30-17:00 h. Chair: Marta Martínez Júlvez**

**Biomolecular interactions.**

15:30 - 16:00 **A. Velázquez-Campoy**, 20 years of biological calorimetry at BIFI. Ref. [12PI](#).

16:00 - 16:15 **P.M. García Franco**, Biophysical Characterization of a zinc-dependent Human Histone Deacetylase 8 (HDAC8): A promising Therapeutic Target for Cancer. Ref. [16T](#).

**Clinical diagnosis and drug delivery**

16:15 - 16:30 **S. Hermoso**, First steps for TLB in machine learning systems: diagnosis of pancreatic cancer in a Danish population. Ref. [17T](#).

**External contribution**

16:30 - 17:00 **L.M. Esteban**, A Stepwise Algorithm for Linearly Combining Biomarkers under Youden Index Maximization. Ref. [13PI](#).

**17:00-17:30 h. Coffee Break.**

**Poster Session 2. January 26<sup>th</sup>, 17:30-19:30 h.**

**BIFI council meeting. January 26<sup>th</sup>, 18:30 h. (BIFI members only)**

## Friday, January 27<sup>th</sup>

### Session 7. January 27<sup>th</sup>, 09:00-11:00 h. Chair: Joaquín Sanz

#### Group of Theoretic and advanced modeling.

- 09:00 - 09:30 **P. Valgañón**, Contagion-diffusion processes with recurrent mobility patterns of distinguishable agents and control strategies. Ref. [18T](#).  
09:30 - 09:45 **H. Pérez**, Dynamics of opinion polarization in weighted graphs. Ref. [19T](#).

#### External contribution

- 09:45 - 10:00 **A. Nicolas**, Assessment of the Risks of Viral Transmission in a Crowd: Combining Observations of the Interactions between Pedestrians in Daily-Life Situations and Fluid-Dynamical Simulations. Ref. [14PI](#).

#### Complex systems and networks lab.

- 10:00 - 10:30 **A. Aleta**, A need for a paradigm shift in healthy nutrition research. Ref. [15PI](#).  
10:30 - 10:45 **A. de Miguel**, Exploring the integration of micro-mobility and epidemic models: d-EPR + SIR. Ref. [20T](#).  
10:45 - 11:00 **M. Tovar**, Modelling decisions influence the impact estimates of new Tuberculosis vaccines: The case of China. Ref. [21T](#).

### 11:00-11:30 h. Coffee Break

### Session 8. January 27<sup>th</sup>, 11:30-13:30 h. Chair: Pilar Catalán

#### Protein folding and molecular design.

- 11:30 - 12:00 **J. Sancho**, Molecular interactions and forces that make proteins stable: an inventory from atomistic MD simulations. Ref. [16PI](#).  
12:00 - 12:15 **P. Bruñén**, Design and synthesis of FMN derivatives for covalent binding to *Anabaena* apoflavodoxin. Ref. [22T](#).  
12:15 - 12:30 **J.J. Galano-Frutos**, Integrating Experiments and MD Simulations for Modeling the Structural Ensemble of a Protein Molten Globule: the *Helicobacter pylori* apoflavodoxin at acidic pH. Ref. [23T](#).  
12:30 - 12:45 **R. Maity**, Multi-OMICs for antibacterial mode of action determination. Ref. [24T](#).

#### Genetic regulation and physiology of cyanobacteria.

- 12:45 - 13:15 **M. Fillat**, Regulatory networks operated by FUR (ferric uptake regulator) proteins in *Anabaena* sp. PCC7120. Ref. [17PI](#).  
13:15 - 13:30 **J Guio**, Shedding light on novel transcriptional regulatory networks in the cyanobacterium *Anabaena* sp. PCC7120. Ref. [25T](#).

### 13:30-15:30 h. Lunch Break.

**Session 9. January 27th, 15:30-16:30 h. Chair: María Fillat**

**Plant evolutionary and genetic biology.**

- 15:30 - 16:00 **P. Catalán**, 20<sup>th</sup> anniversary of model grasses, study systems of evolutionary and functional diversity of monocots. Ref. [18Pi](#)
- 16:00 - 16:15 **M. Campos**, Unveiling the origins of the overlooked model grasses *Brachypodium stacei* and *B. hybridum*. Ref. [26T](#).
- 16:15 - 16:30 **R. Sancho**, Evolution and dynamics of the repeatome and its transposons in the temperate grass model genus *Brachypodium*. Ref. [27T](#).

**16:30 h. Closing remarks & poster prizes.**