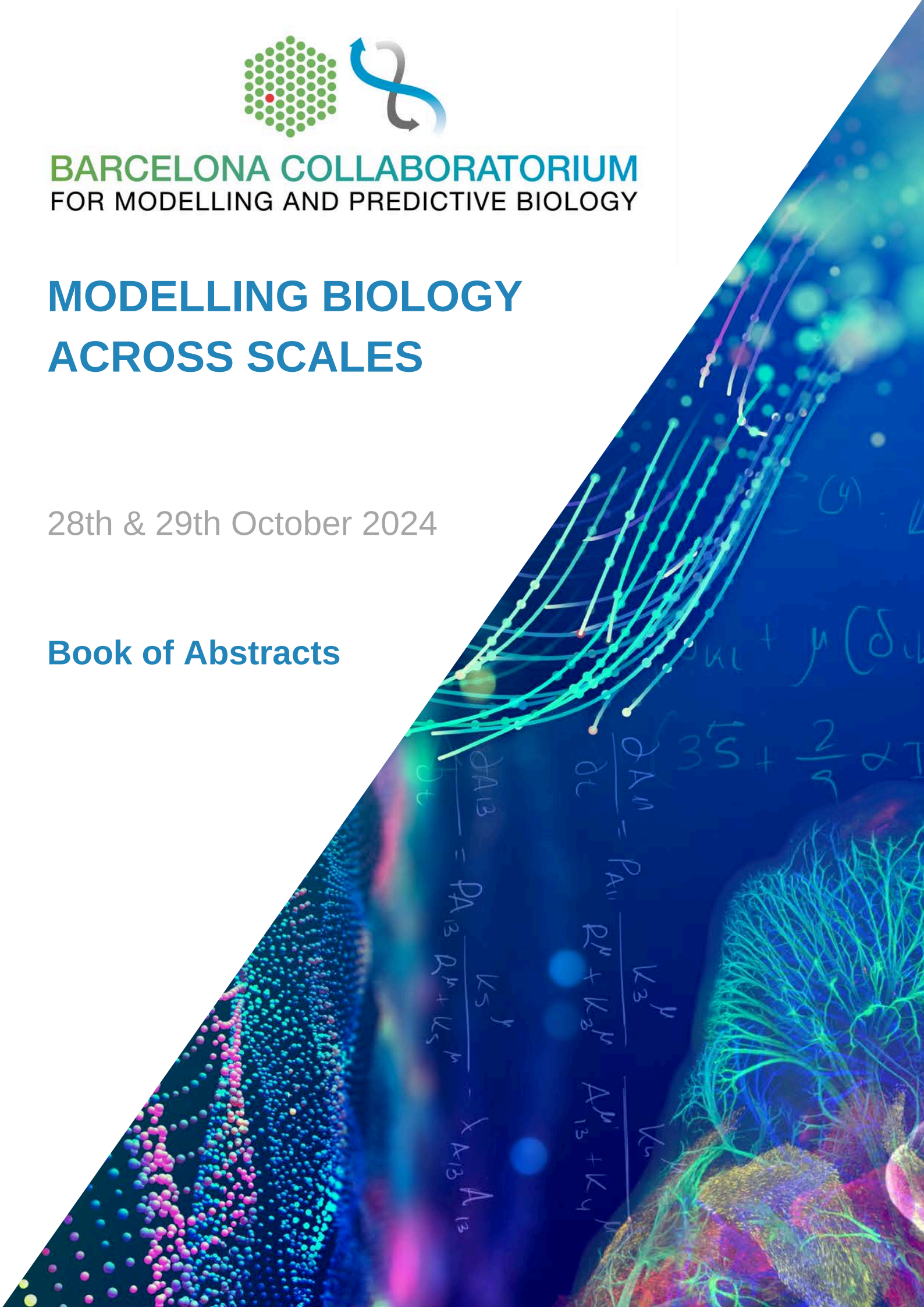
BARCELONA COLLABORATORIUM
FOR MODELLING AND PREDICTIVE BIOLOGY

# MODELLING BIOLOGY ACROSS SCALES

28th & 29th October 2024

## Book of Abstracts



# SUPPORTED BY:


# FUNDERS:



# PROGRAM

## DAY 1 - OCTOBER 28th

09:00 Registration

09:30 Welcome and presentation by Scientific Organizers
**Nora Martin** and **Rosa Martinez Corral**

Session I: Mathematical models for biological complexity
*Chair:* ***Nora Martin***

09:40 **"Chromosomes as communication and memory machines"**
**Leonid Mirny** | Massachusetts Institute of Technology (MIT)

10:20 **"Topology for spatio-temporal biology"**
**Heather Harrington** | Max Planck Institute of Molecular Cell Biology and Genetics

11:00 *Coffee break*

11:30 **"Models with enhanced predictive power for systems and synthetic biology"**
**Irene Otero-Muras** | Institute for Integrative Systems Biology

12:10 Flash talks session I

12:45 *Lunch*

13:30 Poster session I

# PROGRAM

## DAY 1 - OCTOBER 28th

Session II: Development, patterning and tissues
Chair: **James Sharpe**

14:45 **"Processing precise developmental signals: information concepts in gene regulation"**
**Marianne Bauer** | Processing precise developmental signals: information concepts in gene regulation

15:25 **"Positional information theory"**
**Karen Page** | University College London (UCL)

16:05 *Coffee break*

16:40 **"Modularity of the segmentation clock and morphogenesis"**
**Berta Verd** | University of Oxford

17:20 **"Bottom-up mechanobiology: from cell sheets to organoids"**
**Xavier Trepat** | Institute for Bioengineering of Catalonia (IBEC)

18:00 Visit to the Collaboratorium and Networking Drinks

# PROGRAM

## DAY 2 - OCTOBER 29th

9:00 Late registration

Session III: High-dimensional spaces in evolution and populations

*Chair:* ***Rosa Martinez Corral***

09:30 **"Computational modelling of tuberculosis at different scales: from bacillus-macrophage interactions and lung-level dynamics to country-level epidemiology"**

**Clara Prats** | Universitat Politècnica de Catalunya (UPC)

10:10 **“From mutational effects to evolutionary processes: modelling variation with genotype-phenotype maps”**

**Nora Martin** | Barcelona Collaboratorium Independent Fellow, Centre for Genomic Regulation (CRG)

10:50 *Coffee break*

11:20 **"Mutate everything: mapping the energetic and allosteric landscapes of proteins at scale"**

**Ben Lehner** | Centre for Genomic Regulation (CRG), Sanger Institute

# PROGRAM

**DAY 2 - OCTOBER 29th**

12:00 **"Signatures of emergent low-dimensional dynamics in high-throughput biological data"**
**Ilya Nemenman** | Emory University

12:40 Flash talks session II

13:15 *Lunch*

14:00 Poster session II

*Session IV*: Machine learning
*Chair:* ***Nicholas Stroustrup***

15:30 **"Mapping regulatory circuits with AI models - from variants to dysregulation in disease"**
**Olga Troyanskaya** | Princeton University

16:10 **"Knowledge-based machine learning to extract molecular mechanisms from omics data"**
**Julio Saez-Rodriguez** | Heidelberg University

16:50 **Wrap up and final remarks**

# FLASH TALK PROGRAM

**DAY 1 - OCTOBER 28th**

**Start:** 12:10

**"The Stochastic-Thermodynamics of motor proteins: from internal viscosity and ion-motive-force transformation into torque using single-molecule experiments"**
**Jared Lopez Alanilla** | Universite Montpellier

**"Interplay of chromatin organization and mechanics of the cell nucleus"**
**Marco de Corato** | Universidad de Zaragoza

**"Nonequilibrium Antigen Recognition during Infections and Vaccinations"**
**Roberto Morán-Tovar** | Institute for Biological Physics / University of Cologne

**"Multi-Scale Mathematical Modelling of Pancreatic Cancer-Stromal Crosstalk "**
**Jayathilake Pahala Gedara** | Cancer Research UK Scotland Institute

**"Investigating the dynamics of protein constraint across the tree of life with deep Bayesian hierarchical models"**
**Charlie Pugh** | CRG

**"Ants, phase transitions, and how to get into Camp Nou efficiently"**
**Maria Bruna** | University of Oxford

# FLASH TALK PROGRAM

**DAY 1 - OCTOBER 28th**

**"Numerical investigation of the effect of disease-induced red blood cell stiffness on wall shear stress in the microvasculature"**
**Claire Denham** | University of Edinburgh

**"Dynamics of growth, collision, and cell division in epithelial monolayers"**
**Carles Falcó** | University of Oxford

**"Proteins evolve structural robustness to cope with locally chaotic folding landscape as predicted by ESMfold"**
**Samuel von der Dunk** | University of Oxford

**Finish:**
12:45

**“Interplay between phototaxis and photokinesis in light-driven E. coli"**
**Giacomo Frangipane** | Sapienza University of Rome

# FLASH TALK PROGRAM

**DAY 2 - OCTOBER 29th**

**Start:** 12:40

**“Integrative Modeling of Synthetic Biology Interventions in Maize and Rice: From Gene Expression to Whole-Plant Phenotypes”**
**Rui Alves** | Universitat de Lleida

**“CellBasedModels.jl: A generalistic framework for cell-based modelling”**
**Gabriel Torregrosa Cortés** | Universitat Pompeu Fabra

**“PhysiBoSS: Advancing the Path to Digital Twins with Multiscale Modelling”**
**Arnau Montagud** | Institute for Integrative Systems Biology (I2SysBio), CSIC-UV

**"Exploring Vascular Remodelling Across Scales in Limb Development"**
**Giovanni Dalmasso** | IQS - Ramon Llull University

**"Mitotic motor designs determine their ability to organize dynamic microtubules into a minimal bipolar spindle"**
**Wei Xiang Chew** | CRG

**"Mathematical modelling of mechanical communication between cells"**
**Juan Arellano Tintó** | Centre de Reserca Matematica

# FLASH TALK PROGRAM

**DAY 2 - OCTOBER 29th**

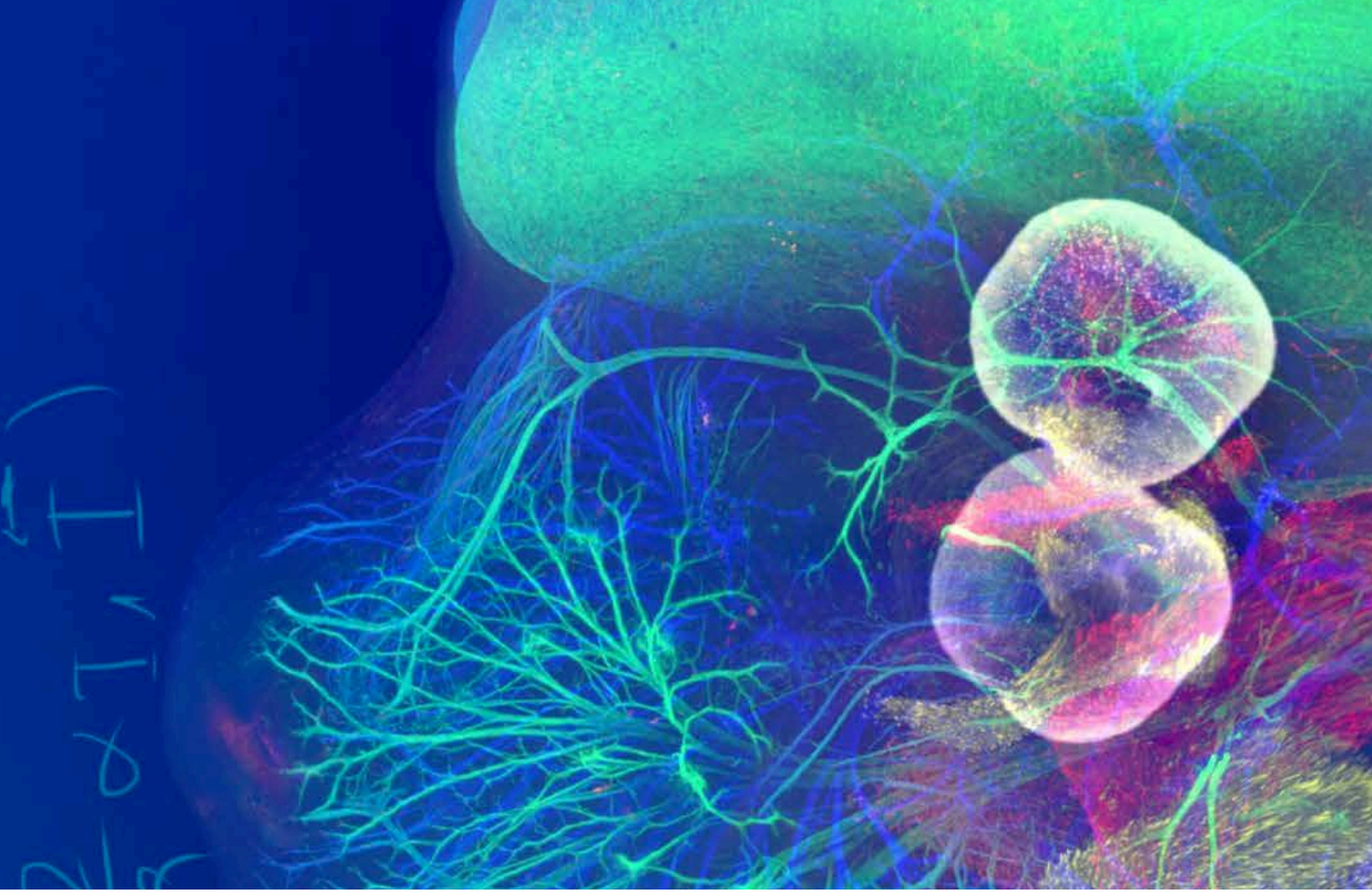
**"Boundary geometry controls topological defect transitions that determine lumen nucleation in embryonic development"**
**Pamela Guruciaga** | EMBL

**"Understanding feedback control in biological systems"**
**Mariana Gómez Schiavon** | LIIGH, UNAM

**"Mathematical model reveals rate-limiting step in neurodegenerative disease from patient data."**
**Georg Meisl** | University of Cambridge

**“From 2D live-cell images to a 3D model: how to get structural information in living cells"**
**Altair Chinchilla Hernandez** | MELIS-UPF

**Finish:**
13:15



# Speakers

# LEONID A. MIRNY

Institute for Medical Engineering & Science at MIT

## *“Chromosomes as communication and memory machines”*

Chromosomes are long polymers of genomic DNA decorated with proteins. We are interested in understanding how cells fold chromosomes to read, write, and process genetic and epigenetic information. Could the way chromosomes are folded carry information itself? Recent works from my group and others have shown that chromosomes function as active polymers. First, we discovered that chromosomes are folded by the ATP-dependent process of loop extrusion, where molecular motors form progressively larger loops. This collective action of nanometer-sized motors shapes micro-sized chromosomes. We demonstrated how this mechanism can also establish complex long-range communication between regulatory elements and genes. Second, we found that chromosome folding plays a key role in storing "epigenetic memory," which refers to patterns of chemical marks along the genome. Although these marks are subject to loss and spreading by enzymes, when genome folding is influenced by the marks, the pattern can be preserved for hundreds of cell divisions.

We also identified a parallel between this mechanism of epigenetic memory and associative memory in neural networks, suggesting that this system may be capable of performing more complex information-processing tasks.

# Nora Martin

Barcelona Collaboratorium Independent Fellow, CRG

## *“From mutational effects to evolutionary processes: modelling variation with genotype-phenotype maps”*

For quantitative models of evolutionary processes, variation is a key ingredient: new phenotypes must first be introduced as variation through random mutations, before selection can act on them. Variation is complex to model since the phenotypic effect of a mutation depends on many biological processes, and the same mutation may have a different phenotypic effect when applied to different genotypes. This complexity can be approached systematically with the framework of genotype-phenotype (GP) maps: if each possible genotype is mapped to a phenotype, we can translate genotypic mutations into phenotypic changes, whether the phenotype is a molecular structure or a growth pattern. By working in the abstract framework of GP maps, we can start with a simple system, for example RNA secondary structure phenotypes, which can be modelled exhaustively with computational tools. Then the insights from such simple systems can be applied to more complex examples. Thus, in this talk, I will highlight key GP map properties, and discuss their implications for evolutionary processes.

# Ben Lehner

CRG/Sanger

## *“Mutate everything: mapping the energetic and allosteric landscapes of proteins at scale”*

The objective of the new Generative and Synthetic Genomics program at the Wellcome Sanger Institute is to produce foundational methods, datasets and models to help transform molecular biology into a predictive engineering science. Towards this goal we have developed methods that combine mutagenesis with model fitting using machine learning to quantify the effects of millions of sequence variants on the properties of proteins and RNAs, including protein stability, aggregation and binding affinities. This has allowed us to produce the first comprehensive maps of allosteric communication in proteins. Thousands of proteins have now been genetically-validated as therapeutic targets in hundreds of human diseases. However, very few have actually been successfully targeted and many are considered ‘undruggable’. This is particularly true for proteins that function via protein-protein interactions: direct inhibition of binding interfaces is difficult, requiring the identification of allosteric sites. However, most proteins have no known allosteric sites and a comprehensive allosteric map does not exist for any protein.

We have addressed this shortcoming by charting multiple global atlases of inhibitory allosteric communication in KRAS, a protein mutated in 1 in 10 human cancers.We quantified the impact of >26,000 mutations on the folding of KRAS and its binding to six interaction partners. Genetic interactions in double mutants allowed us to perform biophysical measurements at scale, inferring >22,000 causal free energy changes, a similar number of measurements as the total made for proteins to date. These energy landscapes quantify how mutations tune the binding specificity of a signalling protein and map the inhibitory allosteric sites for an important therapeutic target. Allosteric mutations typically inhibit binding to all tested effectors but they can also change the binding specificity, revealing the regulatory, evolutionary and therapeutic potential to tune pathway activation. It should be possible to comprehensively identify allosteric target sites in many important proteins and learn how to accurately predict allostery and other protein properties from sequence.

# Irene Otero-Muras

I2SysBio

## *“Models with enhanced predictive power for systems and synthetic biology”*

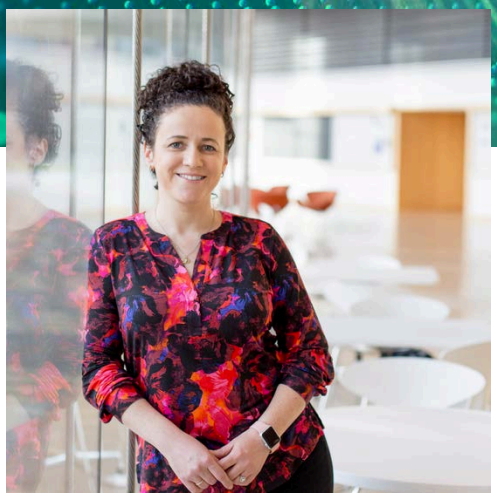
Mathematical models play a crucial role in understanding biological processes and systems by providing insights into the underlying mechanisms and their dynamics. However, significant challenges often arise in making accurate predictions of future behavior based on a set of designated inputs. In the context of model-based design of biomolecular circuits, predictability refers to the ability to forecast the cellular behaviour using models that capture the available knowledge on properties of circuit logic, parts and host cell. Despite significant advances mainly in the design based on logic gates and steady state input-output behaviours we are still far from achieving precision biocircuit engineering for the increasingly complex functionalities required by cutting-edge synthetic biology applications. In this talk, we will explore advanced modelling techniques and frameworks to address current limitations, and discuss how these can be applied to the precision engineering, analysis, and control of biological systems. Specifically, we will elaborate on the engineering of bistable and bimodal switches for precision engineering of cell cognition capabilities in presence of different levels of molecular noise.

# Julio Saez-Rodriguez

Heidelberg University

## *“Knowledge-based machine learning to extract molecular mechanisms from omics data”*

Omics approaches, in particular those with single-cell and spatial resolution, provide unique opportunities to study intra- and inter-cellular processes using computational approaches. The use of prior biological knowledge allows us to reduce the dimensionality and increase the interpretability of the data, in particular by extracting from the data features describing the activity of molecular processes such as signalling pathways, gene regulatory networks, and cell-cell communication events. These approaches allow us to identify key processes, that can be in turn studied in detailed with dynamic mechanistic models. As these computational approaches are further developed, and tailored to the ever-increasing coverage and resolution of mics technologies, we can develop mechanistic and predictive models of cellular and tissue processes. These models may in turn be powerful tools to understand physiological processes, and their deregulation in diseases.

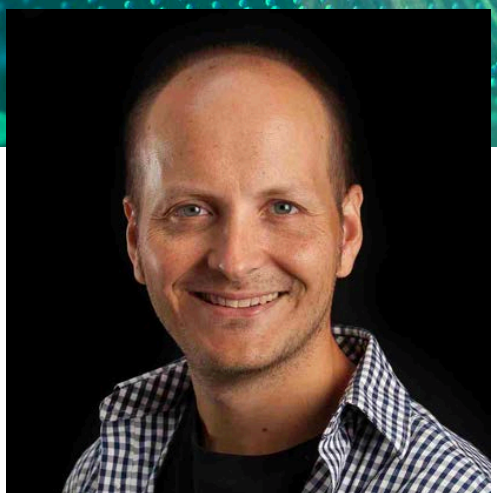


# Olga Troyanskaya

Princeton University

## *“Mapping regulatory circuits with AI models - from variants to dysregulation in disease”*

This talk will address a key challenge in biomedical science - development of a complete understanding of the genomic architecture of disease. The increasingly wide availability of genomic data (including from whole genome sequencing and -omics approaches) has far outpaced our ability to analyze these datasets. Challenges include interpreting the 98% of the genome that is noncoding, detangling genomic signals regulating cell-type-specific gene expression and splicing, and mapping disease-associated cellular circuits from multi-omic datasets. I will discuss AI/ML approaches that we have developed to address these challenges, and present their applications to autism, cancer, and infections. These methods are accessible to researchers through user-friendly interface humanbase.io.



# Xavier Trepat

IBEC

## *“Bottom-up mechanobiology: from cell sheets to organoids”*

Epithelial sheets form specialized 3D structures suited to their physiological roles, such as branched alveoli in the lungs, tubes in the kidney, and villi in the intestine. To generate and maintain these structures, epithelia must undergo complex 3D deformations across length and time scales. How epithelial shape arises from active stresses, viscoelasticity and luminal pressure remains poorly understood. I will present different approaches to study the mechanobiology of epithelial shape from the bottom up. I will discuss new technologies to design epithelia of arbitrary size and geometry and to subject them to controlled mechanical deformations in 3D. I will show that monolayers exhibit superelastic behavior when stretch is applied and that they readily buckle when compressed. We use this phenomenology and a 3D vertex model to rationally direct spontaneous pattern formation, and hence engineer tissue folding. I will also present our recent advances to understand the mechanobiology of intestinal organoids. We show that these organoids exhibit a non-monotonic stress distribution that defines mechanical and functional compartments. Finally, I will discuss how intestinal mechanobiology is derailed in patient-derived colorectal cancer organoids.


## Berta Verd

University of Oxford


# *“Modularity of the segmentation clock and morphogenesis”*


Vertebrates have evolved great diversity in the number of segments dividing the trunk body, however the developmental origin of the evolvability of this trait is poorly understood. The number of segments is thought to be determined in embryogenesis as a product of morphogenesis of the pre-somitic mesoderm (PSM) and the periodicity of a molecular oscillator active within the PSM known as the segmentation clock. Here we explore whether the clock and PSM morphogenesis exhibit developmental modularity, as independent evolution of these two processes may explain the high evolvability of segment number. Using a computational model of the clock and PSM parameterised for zebrafish, we find that the clock is broadly robust to variation in morphogenetic processes such as cell ingression, motility, compaction, and cell division. We show that this robustness is in part determined by the length of the PSM and the strength of phase coupling in the clock. As previous studies report no changes to morphogenesis upon perturbing the clock, we suggest that the clock and morphogenesis of the PSM exhibit developmental modularity.


## Clara Prats Soler

Universitat Politècnica de Catalunya


# *"Computational modelling of tuberculosis at different scales: from bacillus-macrophage interactions and lung-level dynamics to country-level epidemiology"*

Tuberculosis (TB) is an infectious disease caused by Mycobacterium tuberculosis (Mtb) that has accompanied humanity since prehistory, still causing more than 1.5 million deaths annually. Understanding complex interactions and dynamics of TB across various spatio-temporal scales is crucial for advancing our knowledge of its natural history and epidemiology. We employ diverse computational modelling approaches, ranging from dynamical equation-based systems to agent-based models. Our research addresses several key questions, aiming to progressively understand each phenomenon and scale involved. These range from investigating microscopic interactions between Mtb and macrophages in alveolar tissue to exploring endogenous reinfection dynamics through virtual bronchial tree simulations and analysing macroscopic epidemiological patterns.

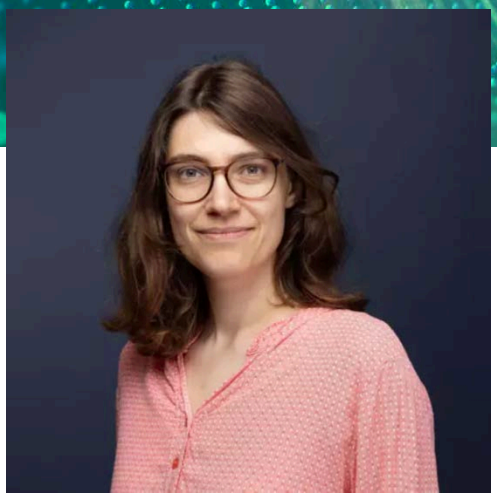
The insights gained from these studies enhance our understanding of TB pathogenesis and progression providing, for instance, essential information for unravelling the factors contributing to the development of active disease in only 10% of infected individuals, or computational tools for improving control programs and combating this persistent disease.

## Heather Harrington

Max Planck Institute of Molecular Cell Biology and Genetics

# *“Topology for spatio-temporal biology”*

Many processes in the life sciences are inherently multi-scale and dynamic. Spatial structures and patterns vary across levels of organisation, from molecular to multi-cellular to multi-organism. With more sophisticated mechanistic models and data available, quantitative tools are needed to study their evolution in space and time. Topological data analysis (TDA) provides a multi-scale summary of data. We review the main tools in topological data analysis and how single and multi-parameter persistent homology provide insights to biological systems.



## Marianne Bauer

TU delft

# *“Processing precise developmental signals: information concepts in gene regulation”*

Cells express genes when they respond to environmental changes, differentiate to different cell fates, or develop into a healthy organism. Gene expression is often regulated by externally supplied cues, such as changing transcription factor concentrations. The expression in response to a changing concentration can be viewed as a type of decision that can be analyzed in terms of an information-theoretic framework. In this talk, I will show, on the examples of early development in the fruit fly and in cultured mouse stem cells, how such an information-theoretic inference approach can help us understand features of a complex signalling apparatus that may be difficult to model, due to the complexity of the contributing regulatory factors. I will introduce how this approach can help us understand features of the fly’s transcriptional apparatus, extending to the architecture of a small enhancer network, as well as the signalling setup in wnt signalling.

# Karen Page

UCL

## *“Positional information theory”*

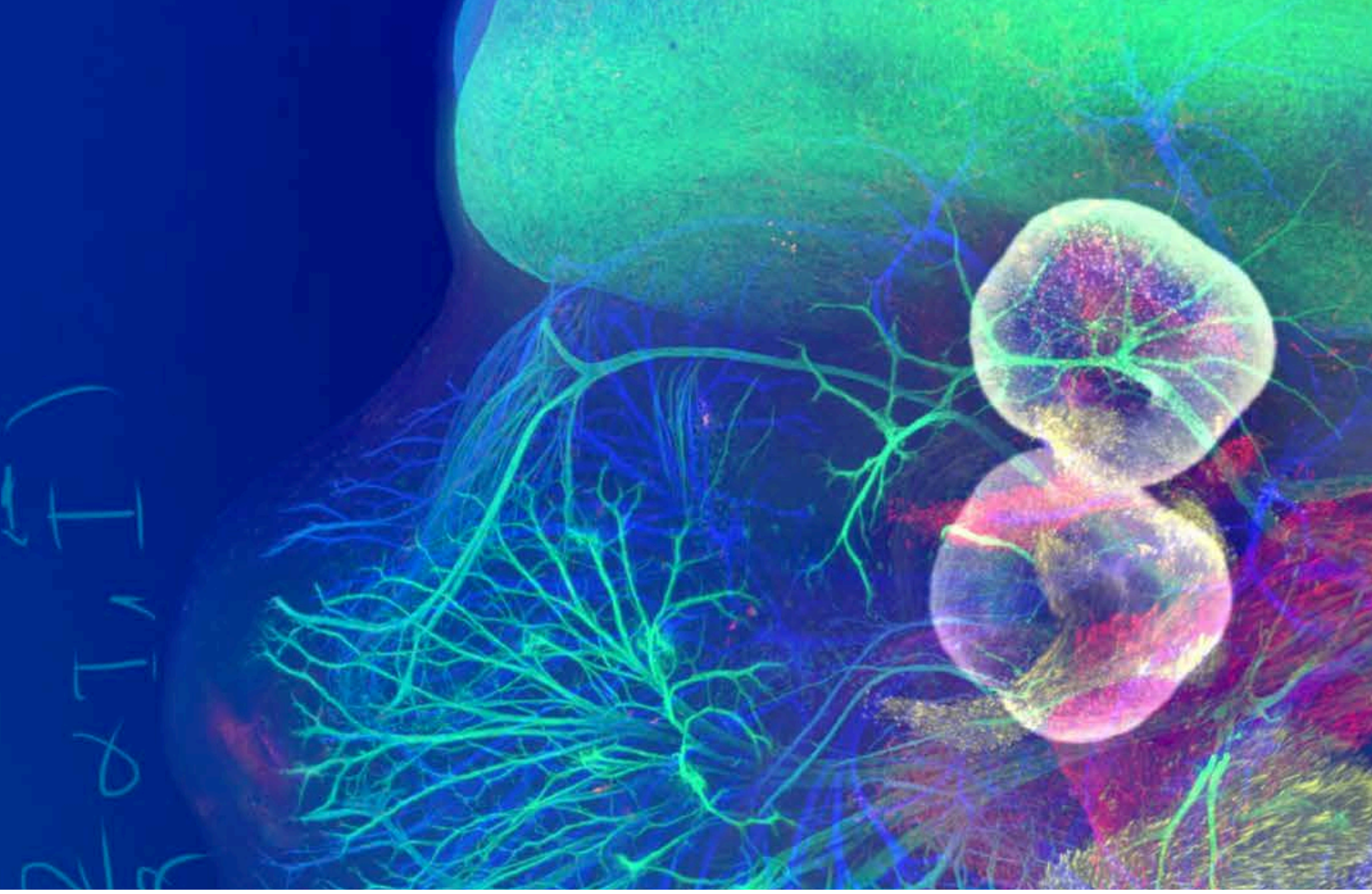
We study the positional information conferred by the morphogens Sonic Hedgehog and BMP in neural tube patterning. We use the mathematics of information theory to quantify the information that cells use to decide their fate. We study the encoding, recoding and decoding that take place as the morphogen gradient is formed, triggers a nuclear response and determines cell fates using a gene regulatory network.


## Ilya Nemenman

Emory University


# *“Signatures of emergent low-dimensional dynamics in high-throughput biological data”*


Modern biological experiments often measure the activity of thousands of components, such as firing patterns of neurons or the frequency of hundreds of genomes in an ecology. These measurements reveal surprising universal features spanning various biological domains, including those a physicist might interpret as signatures of criticality. Focusing on neural population recordings, I will demonstrate how simple models explain these results. A similar analysis applies to other biological and artificial systems (e.g., immunology, large neural networks), and I will briefly touch on these as well. I will argue that the success of these models suggests the emergence of low-dimensional collective dynamics in the studied systems. By identifying these collective degrees of freedom and their interactions, we can hope to develop models of nervous systems without neurons, tissues without cells, and evolution without individuals or genes.



# SELECTED POSTERS

The first poster number corresponds to the assigned stand, and the second number indicates the presentation day.

| Poster | Title | Author | Co-author |
|---|---|---|---|
| **1.1** | Simplicity Bias in Self-Assembling Polyominoes: An Algorithmic Perspective | Prarthana Agrawal | Ard Louis |
| **1.2** | Integrative Modeling of Synthetic Biology Interventions in Maize and Rice: From Gene Expression to Whole-Plant Phenotypes | Rui Alves | Jorge Comas, Oriol Basallo, Abel Lucido, Ester Vilaprinyo, Alberto Marin, Sanguino, Albert Sorribas |
| **2.1** | Observing Wound Healing in vivo: Imaging, Deep-Learning and Projection | Henry Andralojc | - |
| **2.2** | Mathematical modelling of mechanical communication between cells | Juan Arellano Tintó | - |
| **3.1** | LimbLab: Pipeline for Analysis and Visualization of Limb Buds | Laura Aviñó | Heura Cardona, Marco Musy, James Sharpe, Giovanni Dalmasso |
| **3.2** | Energetic portrait of the amyloid beta nucleation transition state | Anna Arutyunyan | Mireia Seuma, Andre J. Faure, Benedetta Bolognesi, Ben Lehner |
| **4.1** | Scaling, ripening and division in emulsions of chemically active droplets | Giacomo Bartolucci | Jonathan Bauermann, Job Boekhoven, Frank Jülicher, Christoph A. Weber |
| **4.2** | Evolutionary-informed latent variable models for genetic disease discovery | Federico Billeci | Sílvia Bonàs-Guarch, Mafalda Dias, Jonathan Frazer |
| **5.1** | Ants, phase transitions, and how to get into Camp Nou efficiently | Maria Bruna | - |

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| **5.2** | Three-dimensional simulations of host-microbiota and microbiota-microbiota interactions | Nikolai Bykov | Bryan Wang, Zoe Horisberger, Marta Contreras, Carlotta Pietroni, Urvish Trivedi, Antton Alberdi, Marc A. Marti-Renom |
| **6.1** | Alternative splicing variability between human populations at single-cell resolution | Rubén Chazarra Gil | Martin Hemberg, Marta Melé |
| **6.2** | Mitotic motor designs determine their ability to organize dynamic microtubules into a minimal bipolar spindle | Wei Xiang Chew | François Nédélec, Thomas Surrey |
| **7.1** | Interplay of chromatin organization and mechanics of the cell nucleus | Marco de Corato | María José Gomez-Benito |
| **7.2** | From 2D live-cell images to a 3D model: how to get structural information in living cells | Altair Chinchilla Hernandez | Laura I. Betancur, Ignacia Echeverria, Andrej Šali, Baldo Oliva, Oriol Gallego |
| **8.1** | VEGF-A differentially influences fibroblast migration and receptor spatiotemporal organization as a function of cell density | Marta Cullell-Dalmau | Marta Otero-Viñas, Montse Masoliver, Joan Bertran, and Carlo Manzo |
| **8.2** | Exploring Vascular Remodelling Across Scales in Limb Development | Giovanni Dalmasso | - |
| **9.1** | Numerical investigation of the effect of disease-induced red blood cell stiffness on wall shear stress in the microvasculature | Claire Denham | Timm Krueger, Miguel O. Bernabeu |
| **9.2** | Learning in single cells: biochemically-plausible models of habituation | Lina Eckert | - |
| **10.1** | Dynamics of growth, collision, and cell division in epithelial monolayers | Carles Falcó | José A. Carrillo , Daniel J. Cohen, Ruth E. Baker |

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| **10.2** | Comprehensive identification of allosteric sites in human kinases | Carla Folgado Salido | Carla Folgado, Toni Beltran, Ben Lehner |
| **11.1** | Interplay between phototaxis and photokinesis in light-driven E. coli | Giacomo Frangipane | - |
| **11.2** | Inferring physiological age from the transcriptome with Raptor | Mirko Francesconi | Romain Bulteau, Victor Cat |
| **12.1** | Long Insertions and Deletions (InDels) contribute both to robustness and evolvability in Genotype-Phenotype maps | Manuela Giraud | Nora S. Martin |
| **12.2** | Understanding feedback control in biological systems | Mariana Gómez Schiavon | - |
| **13.1** | High information fidelity and milli-Kelvin sensitivity in the snake pit organ via proximity to a bifurcation | Isabella Graf | - |
| **13.2** | Boundary geometry controls topological defect transitions that determine lumen nucleation in embryonic development | Pamela Guruciaga | Takafumi Ichikawa, Takashi Hiiragi, Anna Erzberger |
| **14.1** | Building a cancer cell line digital twin for exploring novel treatment strategies | Othmane Hayoun Mya | Arnau Montagud, Alfonso Valencia, Miguel Ponce-de-León |
| **14.2** | Broad Adaptability of Coronavirus Adhesion Revealed from the Complementary Surface Affinity of Membrane and Spikes. | Pablo Ibáñez-Freire | A. B. García-Arribas,D. Carlero, P. Palacios-Alonso, M. Cantero-Reviejo, P. Ares, G. López-Polín, H. Yan, Y. Wang, S. Sarkar, M. Chhowalla, H. M. Oksanen, J. Martín-Benito, P. J. de Pablo, R. Delgado-Buscalioni |

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| **15.1** | Density and Inertia Effects on Two-Dimensional Active Semiflexible Filament Suspensions | Giulia Janzen | - |
| **15.2** | Development of a multiscale model of limb morphogenesis | Tim Liebisch | James Sharpe |
| **16.1** | Cell-size and selection for stress-induced binary cell fusion | Xiaoyuan Liu | George W.A Constable, Jon W Pitchford |
| **16.2** | Dynamics close to a curve of equilibria in a helper virus - defective viral genomes - RNA satellite model | Oriol Llopis Almela | Josep Sardanyés, J. Tomás Lázaro, Santiago F. Elena |
| **17.1** | The Stochastic-Thermodynamics of motor proteins: from internal viscosity and ion-motive-force transformation into torque using single-molecule experiments | Jared Lopez-Alanilla | N-O. Wallisera , J. Palmeria , A. Nordb , and F. Pedacc |
| **17.2** | Assessing the compaction gradient of the cellular nucleus using poroelastic indentation assays with optical tweezers on isolated nucleus and computational validation | Horacio Lopez Menendez | Héctor Zamora-Carreras, Marco Mendívil-Carboni, Alejandro Sáinz-Agost, Fernando Falo, Pedro Roda, Francisco Monroy |
| **18.1** | Mechanistic modelling of Streptococcus pneumoniae population dynamics after vaccine introduction | Leonie Lorenz | Joel Hellewell, Nicholas Croucher, John A. Lees |
| **18.2** | Perturbation of microRNA Gene Regulatory Networks design different Waddington's Epigenetic Landscapes for Neuroendocrine Tumors | Ettolore Luzi | - |

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| **19.1** | Modeling the effects of strigolactone levels on maize root system architecture | Abel Lucido | Johan-Fabian Andrade, Oriol Basallo, Abderrhamane Eleiwa, Alberto Marin-Sanguino, Ester Vilaprinyo, Albert Sorribas, Rui Alves |
| **19.2** | Simplicity bias in a computational model of leaf development explains phylogenetic trends | James Malone | N. Martin, S. von der Dunk , A. Louis |
| **20.1** | Spatially-resolved multiscale models shed light into personalized drug treatments | Alejandro Madrid-Valiente | Alfonso Valencia, Arnau Montagud |
| **20.2** | Mapping the energetic and allosteric landscapes of the PDZ domain family | Aina Martí Aranda | Ben Lehner |
| **21.1** | Modeling of cell-type specific STAT5 signaling response by engineered IL-2 | Quim Martí-Baena | - |
| **21.2** | Deep mutagenesis reveals that RIP kinases require a rate of amyloid formation which is ideal for their activity | Mariano Martín | Benedetta Bolognesi |
| **22.1** | PyMembrane: A flexible framework for efficient simulations of biological membranes | Daniel Matoz | Siyu Li, Monica Olvera de la Cruz, Rastko Sknepnek |
| **22.2** | Ten years of Open Targets: Modelling biology across scales using an industry- academia collaborative model | Ellen McDonagh | - |
| **23.1** | Age-related Changes in Isoform Usage and Association with RNA-binding Protein | Taoyu Mei | Andreas Beyer |

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| **23.2** | Mathematical model reveals rate-limiting step in neurodegenerative disease from patient data. | Georg Meisl | Shih-Huan Huang, Annelies Quaegebeur, Timothy Rittman, Tuomas Knowles, James Rowe and David Klenerman |
| **24.1** | A pharmacological chaperone rescues the expression of the vast majority of pathogenic variants in a G protein-coupled receptor | Taylor Mighell | - |
| **24.2** | PhysiBoSS: Advancing the Path to Digital Twins with Multiscale Modelling | Arnau Montagud | Miguel Ponce-de-Leon, Vincent Noël, Thaleia Ntiniakou, Alejandro Madrid, Jose Estragués, Othmane Hayoun-Mya, Jose Carbonell-Caballero, Annika Meert, Gerard Pradas, Emmanuel Barillot, Laurence Calzone, Alfonso Valencia |
| **25.1** | Nonequilibrium Antigen Recognition during Infections and Vaccinations | Roberto Morán-Tovar | Michael Lässig |
| **25.2** | Understanding and predicting variant effects in synthetic binding proteins | Javier Navarro Delgado | Ben lehner |
| **26.1** | Changes in miRNA secondary structure can predict cancer-related mutations | Yavor Novev | Sebastian E. Ahnert |
| **26.2** | Simplicity Bias in Phenotype Transitions of Seal Teeth | Samantha O'Sullivan | Ard Louis |
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