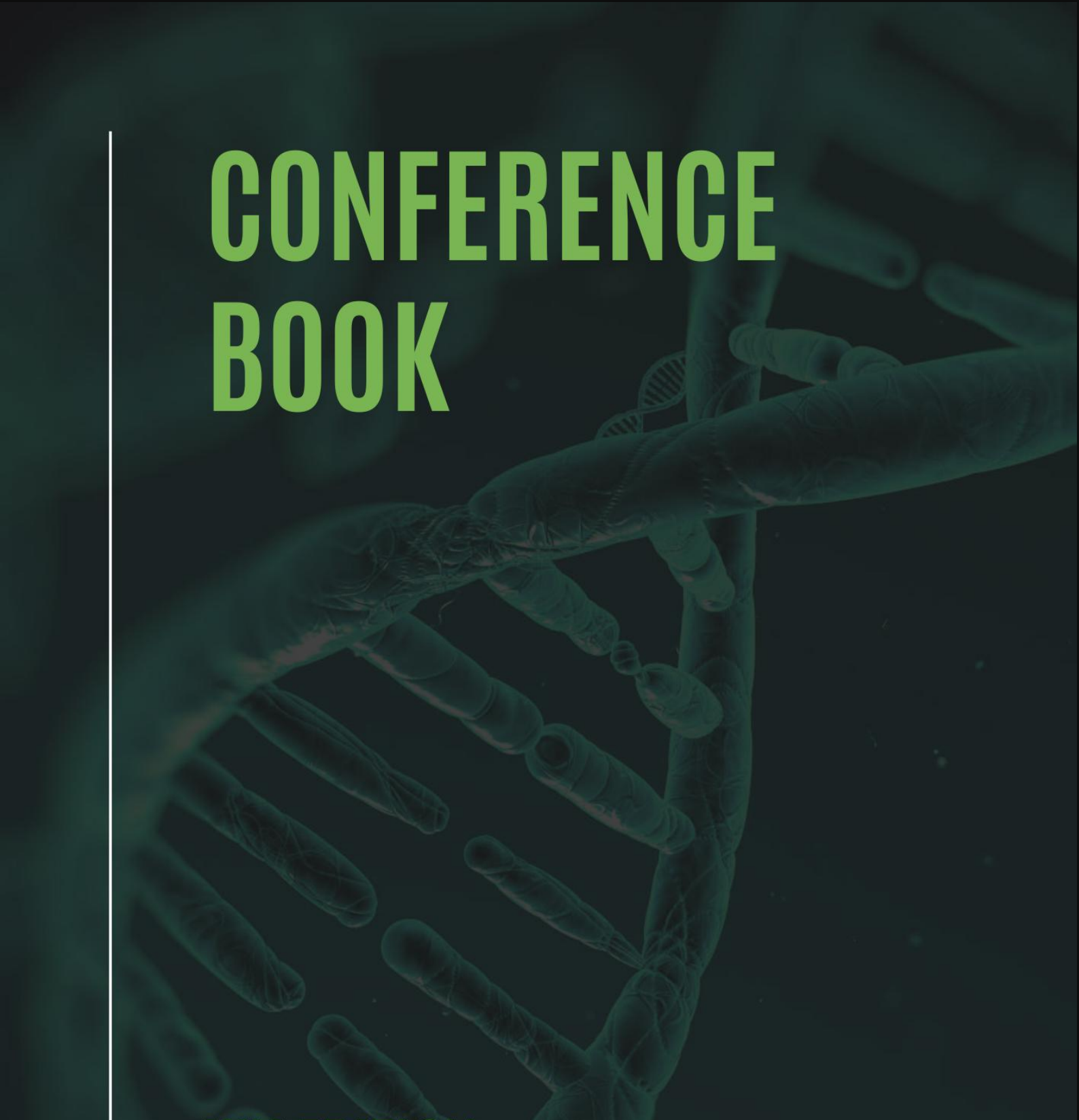
CONFERENCE BOOK



XIV EDITION

26 - 28 MARCH

University of Minho
Gualtar Campus

Bioinformatics
Open Days 2025

Bioinformatics Open Days 2025

WELCOME MESSAGE

Greetings,

It is with great excitement that we welcome you to the XIV Edition of the Bioinformatics Open Days! Since 2012, this student-led initiative has fostered knowledge exchange among students, teachers, and researchers in the fields of Bioinformatics and Computational Biology. This year's event promises to be as dynamic and inspiring as ever.

Our scientific sessions and keynote lectures will cover a diverse range of topics, including the integration of Biology, Chemistry, and Artificial Intelligence to advance personalized pharmacology, the importance of FAIR and Open-Source principles in bioinformatics research software, and cutting-edge developments in bioinformatics methodologies. Discussions will explore how data-driven approaches and machine learning are revolutionizing drug discovery, the role of structured metadata in improving software interoperability, and novel computational strategies for biomedical research.

Beyond these engaging talks, we have also organized three hands-on workshops spanning different applications and backgrounds, as well as innovative oral and poster presentations. Additionally, we are introducing a discussion on the realities of the corporate world, offering valuable insights and guidance for those looking to kick-start their professional journey in Bioinformatics.

We are proud to serve as a platform for knowledge sharing and community building within the Bioinformatics field. We hope this year’s event provides a meaningful and enriching experience for all participants, helping to shape the future of Bioinformatics both nationally and internationally.

Thank you for your participation and enthusiasm—we look forward to welcoming you to the XIV Edition of the Bioinformatics Open Days!

Kind regards,
The Organizing Committee of BOD 2025

Bioinformatics Open Days 2025

THE ORGANIZING COMMITTEE

MIGUEL ROCHA
General Chair

BEATRIZ SANTOS
President

RITA NÓBREGA
Vice-President
Scientific Program

LAÍS CARVALHO
Event Promotion

SOFIA FERREIRA
Event Promotion

DUARTE VELHO
Event Promotion

IAN MACHADO
Event Promotion

RODRIGO ESPERANÇA
Finances

SAMUEL BAPTISTA
Scientific Program

DIOGO ESTEVES
Scientific Program

Bioinformatics Open Days 2025

THE ORGANIZING COMMITTEE

ARMINDO MACHADO
Logistics

RICARDO OLIVEIRA
Logistics

JOÃO FERREIRA
Logistics

FILIPE VASCONCELOS
Logistics

SAMI BENKHELLAT
Logistics

MARIA CARVALHO
Logistics

CATARINA FERNANDES
Logistics

ARTUR GOMES
Logistics

Bioinformatics Open Days 2025

CONTENTS

Bioinformatics Open Days 2025

PROGRAM

MARCH 26TH - WEDNESDAY

09:30 H — Opening Session

10:00 H — Keynote Lecture

Blending Biology, Chemistry and AI to Enable Personalized Systems Pharmacology.

Patrick Aloy

10:45 H — Round Table

BioData.pt "Research Data Management Centres for Living Data: Driving Open Science and Innovation".

Chaired by BioData.pt

12:00 H — Lunch Break

13:45 H — Keynote Lecture

Taking advantage of innovative chemometric tools to unveil vineyard ecosystems and post-bottling dynamics.

Sílvia Rocha

Bioinformatics Open Days 2025

14:30 H — Oral communications [Session 1]

- Mitochondrial Gene Expression Is Independent of Organ Metabolic Rates: Do Cancer Selective Pressures Override the Tumor Microenvironment - **Isabel Duarte**
- The Neighbour Effect: How Interacting Proteins Influence Driver Mutations and Cancer Patient Outcomes - **João Miranda**
- Implementing Metabolic Transformation Algorithms and their application in Ageing-related research - **Bruno Sá**
- Integration of multi-modal datasets to estimate human aging - **Rogério Ribeiro**
- DepMap and GDSC data mining to inform ancestry-driven mechanisms in triple-negative breast cancer - **Ricardo Pinto**

15:45 H — Poser Highlights [Session 1]

Submission nº 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15
*The respective submissions can be checked in the Annex Scientific submissions.

16:00 H — Poster session 1 & Coffee Break

16:45 H — Oral communications [Session 2]

- Guiding computational design for SARS-CoV-2 Spike protein using Molecular Dynamics simulations - **Rita Teixeira**
- Tracing the prevalence and pathogenicity of artifact mutations in ancient Human mitochondrial DNA- **Pedro Fernandes**
- DeepTransyt, annotation of transporter proteins using deep learning - **Gonçalo Apolinário**

Bioinformatics Open Days 2025

- Improving Docking Predictions with a ML-Based Scoring Ensemble - **João Correia**
- Computational Engineering of PETase for Improved PET plastics Substrate Affinity and Degradation Efficiency - **Alexandra Balola**

19:30 H — Meeting

@ Letraria, Braga

20:30 H — Social Dinner and post-dinner activities

@ Taberna do Migaitas, Braga

Bioinformatics Open Days 2025

PROGRAM

MARCH 27TH - THURSDAY

10:00 H	Keynote Lecture The Value FAIR and Open Bioinformatics Research Software **Magnus Palmblad**
10:45 H	Poser Highlights [Session 1] Submission nº 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29 *The respective submissions can be checked in the Annex Scientific submissions.
11:00 H	Poster session 2 & Coffee Break
11:45 H	Oral communications [Session 1]

- Application of bioinformatics in the characterization of multiple aspects of grapevine diversity - **Herlander Azevedo**
- Phylogenomics and functional annotation of 530 non-Saccharomyces yeasts from winemaking environments reveals their fermentome and flavorome- **Ricardo Franco-Duarte**
- Genome-wide characterization of plant resistance genes in cork oak (Quercus suber) - **Luis Gonçalves**
- Eukaryotic Communities and Potential Pathogens in Wastewater Effluents in Ría de Vigo - **Raquel Ríos**
- Deciphering the venoms of Conus species with transcriptomics - **José Morim**

Bioinformatics Open Days 2025

13:00 H	Lunch Break
14:30 H	Keynote Lecture Standardized microbiome data analysis: HPC-ready pipelines from amplicons to MAGs and metagenomics next to real-time metabolic activities **Blaz Stres**
15:15 H	Portuguese Bioinformatics League
16:15 H	Session with Companies Clarivate, Silico Life, OmniunAI, Glintt Global
16:45 H	Job Fair & Coffee Break
17:15 H	Prizes and Closing Session
18:00 H	Social Activities: Quizz @ Carpe Noctem, Braga
19:00 H	Social Activities: BBQ @ Carpe Noctem, Braga

Bioinformatics Open Days 2025

PROGRAM

MARCH 28TH - FRIDAY

9:30 H

Workshops

Software curation in bio.tools

- **Ana Mendes and Mariia Steeghs-Turchina**

Introduction to structural bioinformatic analysis

- **Florencio Pazos**

DeepMol: automating machine learning for computational chemistry

- **João Capela**

Bioinformatics Open Days 2025

SCIENTIFIC SESSIONS AND KEYNOTE LECTURES

Blending Biology, Chemistry and AI to Enable Personalized Systems Pharmacology

Biological data is accumulating at an unprecedented rate, escalating the role of data-driven methods in computational drug discovery. The urge to couple biological data to cutting-edge machine learning has spurred developments in data integration and knowledge representation, especially in the form of heterogeneous, multiplex and semantically-rich biological networks. Today, thanks to the propitious rise in knowledge embedding techniques, these large and complex biological networks can be converted to a vector format that suits the majority of machine learning implementations. In this computational framework, complex connections between entities can be unveiled by means of simple arithmetic operations. Indeed, we demonstrate and experimentally validate that these descriptors can be used to reverse and mimic biological signatures of disease models and genetic perturbations in vitro and in vivo. However, only a tiny fraction of the possible chemical space has been so far explored, meaning that most compounds able to modulate biological activities (i.e. drugs) are yet to be discovered. Thus, we are currently developing strategies to couple bioactivity signatures and generative AI to design new chemical entities with a desired functionality. In particular, we aim at generating cell-specific cytotoxic compounds and new chemical entities (NCEs) to revert the pathological state in complex disorders. All in all, the incorporation of bioactivity descritors generative AI to the drug discovery process is triggering the development of thousands of novel compounds, finally enabling personalized pharmacology.

PATRICK ALOY

As a leading researcher at the Institute for Research in Biomedicine (IRB) in Barcelona, he is dedicated to the development and application of computational models to analyze macromolecular complexes and cellular networks, advancing bioinformatics infrastructure and computational tools for understanding complex biological systems. Aloy's research emphasizes the use of high-resolution 3D structures to explore disease mechanisms, particularly in Alzheimer's and breast cancer.

Bioinformatics Open Days 2025

SCIENTIFIC SESSIONS AND KEYNOTE LECTURES

Standardized microbiome data analysis: HPC-ready pipelines from amplicons to MAGs and metagenomics next to real-time metabolic activities

Planet Earth is a complex system. A grain of soil is a complex system as well in its own. Complex systems operate over large scale differences in time and space and are made of units that interact in nonlinear way to produce emergent properties not possessed by any of the units before. Microbiology has shifted towards analyses of large data sets containing thousands of samples utilizing high performance computing (HPC) coming close to resemble astronomy. The term “Microbiome” contains various layers of information for which there is inherently vague understanding of their information content. Conversely, microbiome information is inherently linked to the vast amount of chemical and physical signatures that change over time and in space in response to variations in thermodynamic conditions of the environment, making them relevant in health and disease. In order to tackle this, machine learning is being increasingly utilized in analyses of data matrices, such as taxonomy, diversity, functional genes, enzymatic reactions, metabolic pathways, metabolomics, environmental chemistry (organic, inorganic), thermodynamic conditions, patient metadata, and other. Large datasets enable extensive biomarker search and mechanistic insight through the adoption of advanced statistics and machine learning approaches that have all revolutionized our established views of health and disease, from operational, diagnostic or mechanistic point of view.

In order to alleviate the bottlenecks and resolve reproducibility issues three HPC compatible pipelines were prepared for the analysis of microbial datasets that include the most cited and already used routines: (i) GUMPP (General Unified Microbiome Profiling Pipeline) takes amplicon sequencing data through Mothur-based taxonomic analyses at four different levels (genus/species/97% operational taxonomic units/amplicon sequence variants), calculates a variety of alpha-diversity indices and inputs BIOM file into Picrust2 for the prediction of microbiome functional genes, enzymatic reactions and metabolic pathways.

(ii) MetaBakery utilizes BioBakery tools for large scale analyses of metagenomics sequencing data and produces species level taxonomy, microbiome functional genes, enzymatic reactions, metabolic pathways and

human gut predicted metabolites. (iii) MAGO (Metagenome Assembled Genomes Orchestra) further extends metagenomics data analysis towards quality control, sequence assembly, binning and evolutionary analysis of metagenome assembled genomes. (iv) GMRC (Gut Microbiome Response Chip) maps the impact of intial conditions and their complex interplay on microbiome physiological responses and resulting chemical space (metabolomic signatures and chemical bonds) in real time streamlined for high-troughput processing.

To facilitate HPC adoption, maximise the use of resources and reproducibility, all pipelines are prepared as Singularity containers with config file that runs the entire pipeline, enables customisation and can be shared with other researchers. The resulting matrices are compatible with modern statistical approaches and machine learning methods to build classification models, search for biomarkers in standardised way on large datasets produced globally in order to improve our understanding of microbiome influence on human health and environment.

BLAZ STRES

Blaz Stres is a bioinformatics researcher specializing in microbial genomics, metagenomics, and systems biology. Based in Slovenia, his work focuses on computational methods for analyzing complex microbial communities, with applications in health, biotechnology, and environmental sciences. He has contributed to the development of bioinformatics tools and workflows that enhance the understanding of microbial functions and interactions. Stres is also involved in advancing FAIR principles and open science initiatives, promoting data accessibility and reproducibility in life sciences research.

Bioinformatics Open Days 2025

SCIENTIFIC SESSIONS AND KEYNOTE LECTURES

The Value FAIR and Open Bioinformatics Research Software

FAIR (Findable, Accessible, Interoperable, and Reusable) principles are essential for ensuring the transparency, reproducibility, and usability of research artefacts. While originally applied to data, the same principles have recently been adopted by the research software community. Beyond FAIR, Free and Open Source Software (FOSS) improves transparency and reusability of the code, with permissive FOSS licenses enabling deployment on high-performance compute infrastructure, and redistribution in workflows and containers.

The ELIXIR bio.tools registry is the largest catalogue of bioinformatics software described using a formal ontology, EDAM, providing rich and machine-readable metadata describing tool functions, input/output data types and formats, license information, publications and more. The EDAM ontology standardizes important bioinformatics concepts and provides a controlled vocabulary for describing software, data and training resources, improving semantic interoperability across ELIXIR Platforms.

By adhering to FAIR and FOSS principles and leveraging structured metadata through resources like bio.tools, bioinformatics software can be more effectively shared, integrated, and maintained, ultimately accelerating scientific discovery and collaboration. In my presentation, I will give concrete examples of projects and services that build on these FOSS and their metadata, including for automated workflow composition and benchmarking.

MAGNUS PALMBLAD

Pioneer in bioinformatics and computational proteomics. His work spans the development and application of computational tools for mass spectrometry-based proteomics and metabolomics, emphasizing FAIR (Findable, Accessible, Interoperable, and Reusable) principles and open-source software. As a senior scientist at the Center for Proteomics and Metabolomics at Leiden University Medical Center, he contributes to advancing bioinformatics infrastructure and automated workflows for biomedical research. Palmblad is also actively involved in the ELIXIR bio.tools registry, helping standardize and improve the accessibility of bioinformatics resources. His editorial work and collaborations within the scientific community support the integration of structured metadata and semantic technologies to enhance interoperability in life sciences research.

Bioinformatics Open Days 2025

SCIENTIFIC SESSIONS AND KEYNOTE LECTURES

Taking advantages of innovative chemometric tools to unveil vineyard ecosystems and post-bottling dynamics

Sustainable viticulture and winemaking continue to represent huge challenges, where better knowledge about the functional role of biodiversity in the vineyard ecosystems is required. The use of advanced methodologies and the combination of several information domains allow the extraction of relevant information about the variables that impact the metabolism of the vine and consequently the characteristics of the grapes and wine. Also, the monitoring of several winemaking and post-bottling steps on wine characteristics has gained interest in recent years, driven by growing interest from researchers and companies to explore, improve, and adapt them to align with market trends and innovation demands. Thus, this talk will focus on the advantages of chemometric tools to process large datasets containing diverse physical-chemical and sensorial data. Specific examples will be selected, namely those that may highlight the application of innovative approaches.

Firstly, it will be discussed the study focused on the understanding of the interactions between climatic conditions, vineyard ecosystem and physicochemical data from a set of Portuguese varieties selected as case study. Combination of ANOVA Simultaneous Component Analysis ASCA+ with linear mixed models (LiMM-PCA) was applied to analyze effect of three factors, harvest, grape variety and vineyard on the physical-chemical parameters and free and glycosidically potential aroma compounds of the grapes. LiMM-PCA allowed to analyze multivariate data set with underlying design, which included both fixed (harvest and cultivar) and random (vineyard) factors. In addition, the approach used allowed to hierarchize the weight of the different variables and to estimate the adaptability of each of the five varieties, which represents a high-value tool in supporting vineyard and wine production management, toward current climate challenges.

Secondly, the relevance of the clustering and variance analysis will be presented to reveal wine differences driven by closure type. The combination of data from diverse analytical techniques unveiled that volatile compound profiling determined by comprehensive two-dimensional gas chromatography (GC×GC) emerged as the most sensitive methodology.

Additionally, the study emphasizes that differences modulated by the wine-closure pairing, which become more pronounced over storage time, can serve as an oenological tool in the construction of the wine identity.

SÍLVIA ROCHA

Leading expert in food biochemistry and metabolomics, specializing in the characterization of plant-derived natural products and agro-food by-products. As an Associate Professor at the University of Aveiro, Portugal, she contributes significantly to the development of advanced chromatographic methodologies for metabolomics studies, focusing on microorganisms, plant-based foods, and human body fluids. Her research emphasizes the sustainable development of innovative food formulations and a deeper understanding of complex biological systems. Rocha is also dedicated to valorizing local agricultural resources, such as Portuguese grape varieties, and applying metabolomics to explore physiological and pathological conditions, like asthma. With over 170 scientific papers, including two books and 17 book chapters, her extensive academic contributions have earned her numerous awards and recognition in the field.

Bioinformatics Open Days 2025

ROUND TABLE

In this roundtable discussion, we will explore the role of Research Data Management (RDM) Centres in fostering a new paradigm for the management of "living data" — dynamic, evolving datasets that require continuous updates, real-time collaboration, and seamless integration across disciplines. As scientific research becomes more data-driven, effective RDM strategies are crucial to ensure data is accessible, interoperable, and reusable, thus facilitating breakthroughs and accelerating innovation.

We will discuss the key challenges facing RDM Centres, including data security, long-term sustainability, and ensuring compliance with the FAIR (Findable, Accessible, Interoperable, and Reusable) principles. Additionally, the conversation will touch on the importance of building infrastructures that support open science, and the potential impact of open, transparent data on research, policy, and industry.

What are the ambitions and next steps for RDM Centres as they evolve to support the growing demands of researchers, the public, and industry stakeholders? Join us as we engage with leading experts in the field to identify both the opportunities and hurdles that come with the management of living data.

BioData.pt

BioData.pt is a national initiative in Portugal dedicated to promoting the efficient management and sharing of research data across scientific disciplines. It aims to provide infrastructure and support for researchers to manage, store, and share their data in compliance with FAIR (Findable, Accessible, Interoperable, and Reusable) principles. By fostering open science, BioData.pt accelerates innovation and facilitates collaboration among researchers, institutions, and industry stakeholders. The platform offers tools, resources, and best practices to help ensure that scientific data is organized, accessible, and leveraged to its full potential, contributing to the advancement of research and technology in the life sciences and beyond.

Bioinformatics Open Days 2025

SCIENTIFIC SUBMISSIONS

ORAL PRESENTATIONS

Nº	Authors	Title
O1	Isabel Duarte	Mitochondrial Gene Expression Is Independent of Organ Metabolic Rates: Do Cancer Selective Pressures Override the Tumor Microenvironment?
O2	João Miranda	The Neighbour Effect: How Interacting Proteins Influence Driver Mutations and Cancer Patient Outcomes
O3	Bruno Sá	Implementing Metabolic Transformation Algorithms and their application in Ageing-related research
O4	Rogério Ribeiro	Integration of multi-modal datasets to estimate human aging
O5	Ricardo Pinto	DepMap and GDSC data mining to inform ancestry-driven mechanisms in triple-negative breast cancer
O6	Rita Teixeira	Guiding computational design for SARS-CoV-2 Spike protein using Molecular Dynamics simulations
O7	Pedro Fernandes	Tracing the prevalence and pathogenicity of artifact mutations in ancient Human mitochondrial DNA
O8	Gonçalo Apolinário	DeepTransyt, annotation of transporter proteins using deep learning
O9	João Correia	Improving Docking Predictions with a ML-Based Scoring Ensemble
O10	Alexandra Balola	Computational Engineering of PETase for Improved PET plastics Substrate Affinity and Degradation Efficiency
O11	Herlander Azevedo	Application of bioinformatics in the characterization of multiple aspects of grapevine diversity
O12	Ricardo Franco-Duarte	Phylogenomics and functional annotation of 530 non-Saccharomyces yeasts from winemaking environments reveals their fermentome and flavorome
O13	Luis Gonçalves	Genome-wide characterization of plant resistance genes in cork oak (Quercus suber)
O14	Raquel Ríos-Castro	Eukaryotic Communities and Potential Pathogens in Wastewater Effluents in Ría de Vigo
O15	José Morim	Deciphering the venoms of Conus species with transcriptomics

Bioinformatics Open Days 2025

SCIENTIFIC SUBMISSIONS

POSTER AND SOFTWARE PRESENTATIONS

Nº	Authors	Title
P1	Gonçalo Sousa	WGCNA as a tool to identify key gene expression networks associated with mistranslation and azole resistance in the human fungal pathogen Candida albicans
P2	Maria Inês Gomes	Benchmarking Causal Reasoning Algorithms for enhanced Drug Discovery: Insights from Clarivate's pre-competitive Algorithm Benchmarking Consortium
P3	Tiago Miranda	Towards a Machine Learning Framework for Predicting MicroRNAs involved in Candidiasis
P4	Diana Silva	Comprehensive Molecular Characterization of Anti-EFG1 2'OMe Effects on C. albicans: A Bioinformatics Study
P5	Inês Carvalho	A machine learning model based on geometric morphometric data for Skeletal Malocclusion diagnosis
P6	Filipa Ferreira	The Diagnosis Network App (DiNA): a computational system for the diagnosis of depressive major disorder
P7	Grigore Platon	Expanding the Kinetic-Regulatory Model of Escherichia coli for High-Value Compound Production from Aromatic Amino Acids
P8	Elias Barreira	Predictability of Genomic Evolution at the Molecular Level
P9	Constança Ilunga	Design and Characterization of MHETase Mutants for Improved PET Degradation: A Combined In Silico and In Vitro Study
P10	Raquel Ríos-Castro	High Throughput sequencing for Monitoring Eukaryotic Pathogens in Castellana WWTP: Insights from the AWARE Project
P11	Rafael Vleira	Introducing AptaCom - A centralized aptamer database
P12	Mahmoud Abdallah	Exploring the Genomic Potential of Macroalgae: A Bioinformatics Pipeline for Protein and Gene Discovery
P13	João Guimarães	Evaluating the Viability of BEAST Software for Accurate Phylogenetic Dating
P14	David Henriques	Enhancing the simulation of anaerobic flux distributions in Saccharomyces cerevisiae using genome-scale metabolic models
P15	Sirine Gaieb	Structural Dynamics of H5N1 Hemagglutinin Globular Head: Insights from Molecular Dynamics Simulations

Bioinformatics Open Days 2025

P16	Sofia Torres	Characterization of tissue immunity in metastatic breast cancer by single-cell RNA-sequencing
P17	Raquel Romão	Akna as a novel RNA-binding protein: uncovering its role in immune cell function through iCLIP-seq analysis
P18	Sofia Ferreira	Understanding lactoferrin multifunctionality by analyzing the full spectrum of its interacting partners and its evolutionary history
P19	Daniela Holdych	Antiphospholipid Syndrome: Insights into the cellular basis of autoimmunity
P20	Mariana Vasques	Characterizing the Heterogeneity and Differentiation of Murine T Follicular Cells using Single-Cell
P21	Bruna Cruz	Decoding Early Neuronal Responses to Injury: A Bioinformatics Approach to Identify Regeneration- Associated Genes
P22	Ana Paulino	The molecular regulatory mechanisms behind the vegetative-to-reproductive transition in Cynara cardunculus
P23	Diana Lourenço	Plastic Biodegradation by Microalgae: Database Development and Sequence Retrieval
P24	Ana Lima	Comprehensive multi-omics database for highly infectious viruses: a focus on HIV, Ebola and SARS-CoV-2
P25	Raquel Domingues	Structural Bioinformatics insights into the stability of a promising RSV-targeting nanobody
P26	André Bagão	Molecular Dynamics Simulations of Glycan Shielding on Prefusion RSV F Protein: Implications for Epitope Accessibility and Vaccine Design
P27	Benedita Pereira	Developing a Repository for the Storage and Analysis of Novel Computationally Designed Proteins
P28	Raquel Ríos-Castro	Behaviour of Infective Stages (L3) of Anisakis simplex in Water Mass and Fish-waste: Transcriptomic Contribution to understanding the Parasite Life Cycle
P29	Elias Barreira	Developing Genomic Models to Predict Breast Cancer Metastatic Progression

If you want to know more about the content of each poster/oral presentation, check out our Abstract Book, available below:

Bioinformatics Open Days 2025

NETWORK SESSION

SESSION WITH COMPANIES

In the Networking Session participants will have the opportunity to interact with each company representative, incentivizing follow-up questions and general discussion about starting their professional career. The aim is to expose successful and growing technological-based companies, whilst closing the gap between company representatives and all those interested.

Clarivate™

SILICOLIFE

Omnium AI

Glintt Global we think tech

Bioinformatics Open Days 2025

WORKSHOPS

SOFTWARE CURATION IN *BIO.TOOLS*

Effective research in bioinformatics and computational biology relies on well-documented and discoverable software. *bio.tools* is a registry of bioinformatics tools that facilitates software discovery, interoperability, and reuse by providing rich, standardized metadata.

This hands-on workshop will provide practical guidance on curating software entries in *bio.tools*. Participants will learn how to improve tool descriptions, add relevant metadata, and contribute new software *to bio.tools*. The session will include collaborative activities to apply these skills in real-world scenarios.

Whether you are a researcher developing bioinformatics tools or a scientist looking for well-documented software for data analysis, this workshop will equip you with the skills to enhance software discoverability and usability through better curation practices.

Ana Mendes (Data Scientist at University of Southern Denmark) and Mariia Steeghs-Turchina (Researcher at UvA & Research software at LUMC).

Bioinformatics Open Days 2025

LEVERAGING ALPHAFOLD AND OTHER PROTEIN STRUCTURE PREDICTION AND ANALYSIS TOOLS FOR OBTAINING BIOLOGICAL INSIGHT

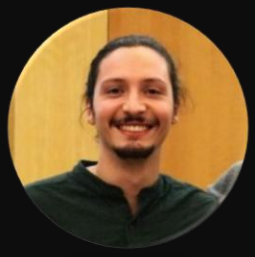
The recently developed AlphaFold system generates three-dimensional structural models of proteins from their amino-acid sequences with accuracy comparable to experimental techniques, achieving a long-sought goal in molecular biology. Together with homology-based modeling and other methods for predicting low-level structural features and analyzing structures, constitute a useful toolbox for molecular biologists, who today have an unprecedented capacity to obtain structural information for their proteins of interest. In this workshop, we will explore the practical usage of AlphaFold and other structure prediction and analysis tools to give an idea of their potential. We will see, using real examples, how to use these programs and interpret the results they produce.

Florencio Pazos (Research Scientist at the National Center for Biotechnology, which is part of the Spanish National Research Council (CSIC), Madrid, Spain).

Bioinformatics Open Days 2025

DEEPMOL: AUTOMATING MACHINE LEARNING FOR COMPUTATIONAL CHEMISTRY

DeepMol is a computational tool designed to streamline tasks for molecular data preprocessing, feature extraction, scaling, selection, and machine learning model training. In this workshop, you will learn to create fast and accurate models for predicting molecular properties. Additionally, we will explore how to use these models to identify the most promising compounds within larger datasets, enhancing your drug discovery and computational chemistry workflows.



João Capela (PhD student at Bioinformatics and Systems Biology research group (BiSBi), in the Centre of Biological Engineering from University of Minho).

Bioinformatics Open Days 2025

SPONSORS AND COLLABORATORS

THANK YOU NOTE

Dear Sponsors, Collaborators, Volunteers, and Members of the Organizing Committee,

On behalf of the XIV Edition of the Bioinformatics Open Days, we extend our heartfelt appreciation for your invaluable support and contributions. Your dedication and hard work were instrumental in making this event a success.

To our sponsors and collaborators—thank you for your generosity and partnership. Your support enabled us to curate a diverse program of keynote talks, workshops, and networking opportunities that were both enriching and inspiring. Your contributions not only helped shape this event but also reinforced its role as a platform that reflects the present and future of the Bioinformatics field.

To our incredible volunteers and organizing committee members, your commitment and tireless efforts in planning and executing this conference did not go unnoticed. Your passion and dedication were the backbone of this event, and we deeply appreciate the time and energy you devoted to ensuring its success.

A special thank you goes to **NEBIUM, the Student Association for Bioinformatics Students at the University of Minho**. Your expertise, dedication, and hands-on involvement in various aspects of the conference were invaluable. Your insights helped shape a program that truly met the needs of all attendees, and we are grateful for your contributions.

We would also like to express our sincere gratitude to **Professor Miguel Rocha, our General Chair**, for his guidance, expertise, and leadership. His insightful advice played a crucial role in steering this event toward success.

The success of this edition of the Bioinformatics Open Days is a testament to the collective efforts of each and every one of you. We are incredibly grateful for your support and look forward to collaborating again in future editions.

Bioinformatics Open Days 2025

SPONSORS AND COLLABORATORS

Universidade do Minho

Thank you!!!

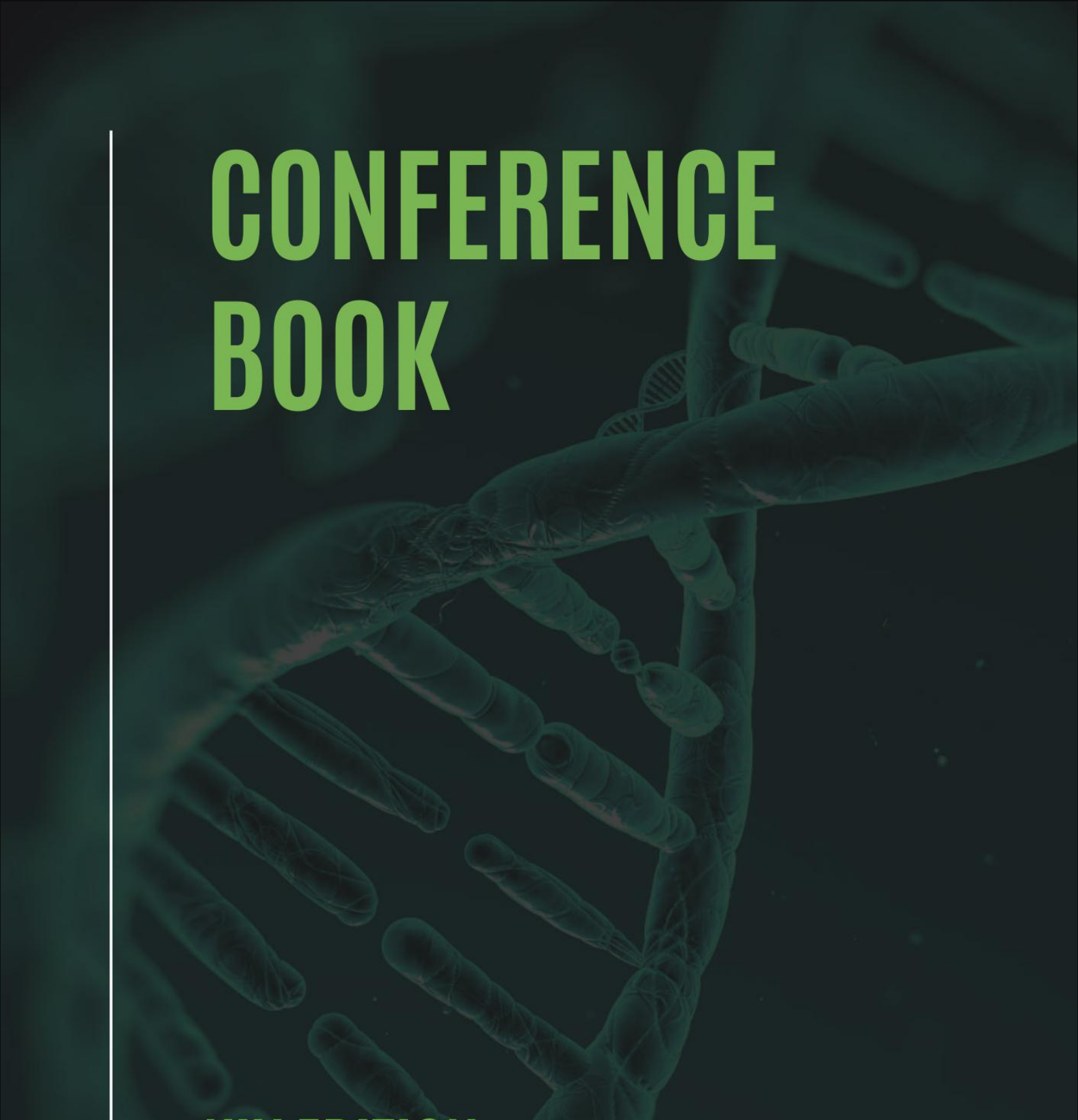
XIV EDITION

Bioinformatics Open Days 2025

Thank you for joining us at XIV BOD!

Your participation and support are greatly appreciated. We look forward to seeing you at future event editions and continuing to grow the Bioinformatics community.

CONFERENCE BOOK



XIV EDITION

26 - 28 MARCH

University of Minho
Gualtar Campus

Bioinformatics
Open Days 2025