

ABSTRACT BOOK

XIV EDITION
26 - 28 MARCH

University of Minho
Gualtar Campus



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 |

O1 - Mitochondrial Gene Expression Is Independent of Organ Metabolic Rates: Do Cancer Selective Pressures Override the Tumor Microenvironment?

Metabolic reprogramming is a recognized hallmark of cancer, playing a crucial role in its initiation and progression. Recent evidence highlights the impact of non-cancer cell metabolism within the tumor microenvironment in modulating tumor development, emphasizing the importance of metabolic factors in understanding cancer biology.

To identify differentially expressed genes (DEGs) in cancer, with a specific focus on mitochondria-located genes, and to compare gene expression profiles between organs with high metabolic-rates (brain, liver, kidneys) and low metabolic-rates (bladder, colon, skin).

RNA-seq data for normal and cancer tissues from the six organs under study were sourced from the GTEx and TCGA databases. The dataset included 2,675 normal tissue samples from GTEx, and 3,633 cancer tissue samples from TCGA. Differential expression analysis was performed using General Linear Models (GLMs), while hierarchical and soft fuzzy clustering were applied to identify distinct gene expression patterns. All analyses were performed in R, and the code is openly accessible in GitHub [<https://github.com/orgs/MitoProfiles/repositories>].

The analysis identified mitochondrial DEGs such as ACSM1, ACSM5, and PRODH, likely reflecting cancer cell adaptations to metabolic and microenvironmental stress. Significant differences in FDX2 (iron-sulfur protein biogenesis) and ACSM2B (free fatty acid activation) suggest the involvement of these pathways in oncogenesis. However, the expression differences were largest between normal and cancer tissues, overshadowing the variation between high and low metabolic-rate organs. Mitochondrial gene expression profiles differ more significantly between cancer and normal tissues than between cancers originating from organs with varying metabolic-rates. This highlights the dominant role of cancer-induced cellular reprogramming over organ-specific microenvironment signals. This raises the hypothesis of a functional convergence of mitochondrial pathways in cancer, particularly those involved in processes such as iron-sulfur cluster biogenesis and fatty acid metabolism, which may be selectively enhanced/suppressed to meet the metabolic demands of cancer cells. This suggests the possibility of a general cancer mitochondrial expression-signature, warranting further investigation.

O2 - The Neighbour Effect: How Interacting Proteins Influence Driver Mutations and Cancer Patient Outcomes

O3 - Implementing Metabolic Transformation Algorithms and their application in Ageing-related research

O4 - Integration of multi-modal datasets to estimate human aging

https://github.com/zroger49/multi_modal_age_prediction

O5 - DepMap and GDSC data mining to inform ancestry-driven mechanisms in triple-negative breast cancer

O6 - Guiding computational design for SARS-CoV-2 Spike protein using Molecular Dynamics simulations

O7 - Tracing the prevalence and pathogenicity of artifact mutations in ancient Human mitochondrial DNA

O8 - DeepTransyt, annotation of transporter proteins using deep learning

<https://github.com/Apolinario8/deeptransyt>

O9 - Improving Docking Predictions with a ML-Based Scoring Ensemble

www.itqb.unl.pt/pm

**O10 - Computational Engineering of PETase for Improved PET plastics
Substrate Affinity and Degradation Efficiency**

O11 - Application of bioinformatics in the characterization of multiple aspects of grapevine diversity

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O12 - Phylogenomics and functional annotation of 530 non-Saccharomyces yeasts from winemaking environments reveals their fermentome and flavorome

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**O13 - Genome-wide characterization of plant resistance genes in cork oak
(*Quercus suber*)**

O14 - Eukaryotic Communities and Potential Pathogens in Wastewater Effluents in Ría de Vigo

O15 - Deciphering the venoms of *Conus* species with transcriptomics

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 <i>Candida albicans</i> |
| 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 <i>C. albicans</i> : 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 <i>Escherichia coli</i> 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 <i>Saccharomyces cerevisiae</i> using genome-scale metabolic models |
| P15 | Sirine Gaieb | Structural Dynamics of H5N1 Hemagglutinin Globular Head: Insights from Molecular Dynamics Simulations |
| P16 | Sofia Torres | Characterization of tissue immunity in metastatic breast cancer by single-cell RNA-sequencing |
| P17 | Raquel Romão | |

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| 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 <i>Cynara cardunculus</i> |
| 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 <i>Anisakis simplex</i> 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 |

P1 - WGCNA as a tool to identify key gene expression networks associated with mistranslation in the human fungal pathogen *Candida albicans*

P2 - Benchmarking Causal Reasoning Algorithms for enhanced Drug Discovery: Insights from Clarivate's pre-competitive Algorithm Benchmarking Consortium

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P4 - Comprehensive Molecular Characterization of Anti-*EFG1* 2'OMe Effects on *C. albicans*: A Bioinformatics Study

P5 - A machine learning model based on geometric morphometric data for Skeletal Malocclusion diagnosis

P6 - The Diagnosis Network App (DiNA): a computational system for the diagnosis of depressive major disorder

P7 - Expanding the Kinetic-Regulatory Model of *Escherichia coli* for High-Value Compound Production from Aromatic Amino Acids

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This work received financial support from the PT national funds (FCT/MECI, Fundação para a Ciência e Tecnologia and Ministério da Educação, Ciência e Inovação) through the project UID/50006 -Laboratório Associado para a Química Verde - Tecnologias e Processos Limpos.

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P12 - Exploring the Genomic Potential of Macroalgae: A Bioinformatics Pipeline for Protein and Gene Discovery

<https://github.com/Mohamedema/ICulture>

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P17 - Akna as a novel RNA-binding protein: uncovering its role in immune cell function through iCLIP-seq analysis

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