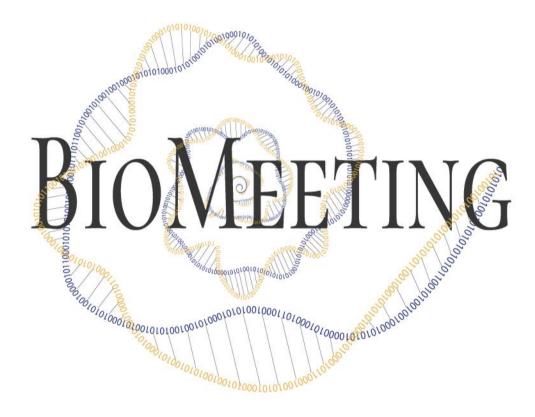
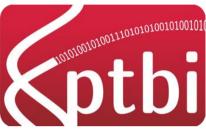
# **BioMeeting 2025**



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## **PRESENTATION ABSTRACTS**

### Attacks on Artificial Intelligence Models and Cybersecurity in Bioinformatics

#### Mateusz Twardawa<sup>1</sup>

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The growing integration of artificial intelligence (AI) into bioinformatics pipelines brings new opportunities for research, diagnostics, and personalized medicine. However, as AI models become essential components of computational biology, they also introduce new security vulnerabilities. This presentation explores the emerging landscape of adversarial threats targeting machine learning models used in bioinformatics, including data poisoning, evasion attacks, and model inversion. Such threats can compromise the integrity of biological data analysis, lead to erroneous predictions and cause data leakage. By highlighting real-world examples and recent research, this talk aims to raise awareness of AI-related security risks and promote a proactive approach to safeguarding AI systems in bioinformatics.

#### **Guess the Structure: A Short Guide to Protein Modeling**

Beata Borysiuk<sup>1</sup> Adam Gruda<sup>1</sup> Sebastian Kraszewski<sup>1</sup>

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Various methods for protein modeling are available nowadays. This work presents a comprehensive guide explaining some of the most popular methods utilized by scientists and some of the basic concepts regarding structural bioinformatics. Furthermore, we show a real-life application of some of the most popular methods and introduce a brief comparison of the obtained results.

Modeling of the 3D protein structures is one of the most important tasks for bioinformaticians, especially when it comes to drug design. In this work, not only do we gather the concise knowledge compendium about protein structure modeling methods, but also provide a comparative study between homology modeling conducted with MODELLER[1] package on the chosen template and structure prediction derived from DeepMind's Alphafold 3 [2] for the TRPV1 non-selective ion channel. This study is an example of how well various methods perform and showcases the possible reliability for computational studies.

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## How to tame the storm in the brain? Technology in the fight against epilepsy

#### Zofia Dobrowolska1

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Epilepsy is a chronic neurological condition characterized by recurrent, unprovoked seizures resulting from abnormal, excessive electrical discharges in the brain. Despite its high global prevalence — affecting approximately 50 million people worldwide — accurate diagnosis and monitoring of epilepsy remain complex due to the unpredictable and heterogeneous nature of seizures. One of the gold standards in clinical and research contexts for seizure detection and characterization is video-electroencephalography (video-EEG), a modality that combines continuous EEG recordings with synchronized video footage of the patient. This integrated approach allows clinicians to correlate electrographic patterns with behavioral manifestations, facilitating more accurate localization and classification of epileptic events.

We aim to provide a pop-scientific yet technically grounded overview of the signal processing techniques used in video-EEG-based seizure detection and analysis. Beginning with an introduction to the physiological basis of seizures and the principles of EEG signal acquisition, we illustrate how seizure activity appears in raw EEG signals — often in the form of sharp spikes, rhythmic discharges, or sudden amplitude changes. However, EEG data are notoriously noisy, often contaminated by motion artifacts, muscle activity, and environmental interference. Signal processing is thus essential for filtering, artifact rejection, and highlighting diagnostically relevant features. We further discuss how machine learning techniques are increasingly being applied to EEG data for automated seizure detection and even forecasting. Supervised algorithms can be trained on labeled datasets to recognize seizure patterns, while deep learning models — such as convolutional neural networks (CNNs) and recurrent neural networks (RNNs) — are showing promise in learning complex temporal dependencies within EEG time series. In parallel, advancements in wearable EEG systems and cloud-based analysis pipelines are bringing these technologies closer to real-world deployment, potentially enabling ambulatory and at-home seizure monitoring.

The integration of video in video-EEG adds another critical layer of information: it allows the classification of clinical versus subclinical events, differentiation from psychogenic non-epileptic seizures (PNES), and contextual understanding of patient behavior. By synchronizing EEG data with time-stamped video, clinicians can determine whether observed physical events align with electrographic changes, increasing diagnostic confidence. As technology continues to evolve, video-EEG and its associated analytical methods stand at the forefront of precision neurology, offering new hope for millions living with epilepsy.

#### How to use bioinformatics to find the laws of biology?

#### Tomasz Kościółek1

<sup>1</sup>Sano Centre for Computational Medicine, Krakow, Poland

It's common knowledge now that the microbiome, in particular the human gut microbiome, is important in health. Gut microbes aid food digestion may regulate immune response and are liked with a plethora of diseases ranging directly from the gut, e.g. obesity, inflammatory bowel disease; through conditions like diabetes; all the way to diseases supposedly far removed from the gut, like Parkinson's, anxiety, depression or schizophrenia. It is however a vast, diverse and dynamic ecosystem composed of trillions of microbial cells and encoding millions of unique genes. This complexity combined with a clearly established potential of the microbiome in biotechnology and medicine poses a unique opportunity for bioinformatics. In my talk, I will describe the methodological approach taken by the Structural and Functional Genomics group at Sano which addresses the most prevalent problems in dealing with microbiome data - multidimensionality, sparsity, compositionality, and batch effects. And how the quest for establishing how the microbiome human health is getting us closer to establishing further laws of biology.

#### Identifying trans-homologous chromatin interactions

Aleksander Jankowski<sup>1</sup> Magdalena A. Machnicka<sup>1</sup>

<sup>1</sup>Faculty of Mathematics, Informatics and Mechanics, University of Warsaw

Interactions between chromosomes forming homologous pairs are known to be widespread in the fruit fly Drosophila melanogaster and present in other organisms. While these trans-homologous interactions affect regulation of gene expression, many details regarding their location, function and mechanisms of action are still unknown. The increased availability of phased Hi-C datasets made it possible to reliably infer such interactions.

We developed a tool called TransContactHiC to detect trans-homologous chromatin interactions in phased Hi-C data and we used it to re-analyze published in situ Hi-C data for heterozygotic Drosophila melanogaster cells. We further assessed the frequency of cis- and trans-homologous interactions for equally sized genomic bins, and detected triads of genomic elements which exhibit significantly different frequency of trans-homologous interactions compared to the cis-homologous counterpart.

We show that triads of genomic elements exhibiting significantly higher frequency of transhomologous interactions are characterized by their clustering within broader regulatory regions, proximity to DNase-seq peaks and presence of disrupted transcription factor motifs at the affected locus. We also show examples of annotated active cis-regulatory modules which might be affected.

## Innovating Drug Discovery: Tackling Challenges and Advancing Treatment Solutions

#### Jacek Kędzierski1

#### <sup>1</sup>Adamed Pharma S.A. Drug Discovery and Early Development Department

Modern approaches to therapeutic protein design and integrated molecular simulations—open new avenues for understanding and engineering the biological mechanisms of drugs. Research in this area has the potential to fill significant gaps in our structural and functional knowledge of proteins and to create entirely new classes of therapeutics that address unmet medical needs.

Despite their promise, these studies face considerable challenges. These include limited predictability of designed protein success, difficulties in optimizing biophysical properties, and the risk of side effects. Additionally, predictive methods are not yet fully aligned with experimental in vitro and in vivo results. Overcoming these hurdles requires the integration of computational and experimental workflows, the development of algorithms that better model biological complexity, and iterative, feedback-driven optimization strategies.

The outcomes of this research have the potential to significantly influence the development of novel drug candidates threw advancements in computational chemistry, bioinformatics, biotechnology, and bioengineering. However, to fully unlock this potential, robust validation protocols are needed. Demonstrating the predictive accuracy and applicability domain of these models is essential to ensure confidence in their application across different research stage and therapeutic contexts. The emphasis must be on systematic benchmarking and validation of computational methods, enabling the development of scalable, adaptable frameworks that support cross-disciplinary collaboration and facilitate effective knowledge transfer between academia and the industry.

## Multimodal analysis of human behavior in relation to disease detection

#### Wojciech Szecówka1

#### <sup>1</sup>Department of of Electrical Engineering, Automation, Computer Science and Biomedical Engineering, AGH University of Krakow

This project presents an innovative approach to using augmented reality technology and machine learning algorithms to diagnose Parkinson's disease. A methodology was developed for the integrated analysis of multimodal data, including body movement, voice and eye tracking trajectories. The data collection process used augmented reality glasses and a dedicated DiagNeuro application (developed as part of the LIDER\* project) to record seventeen separate diagnostic tasks. Data from dozens of healthy individuals and patients with Parkinson's disease were subjected to advanced processing, including normalization, imputation of missing data, outlier detection and multimodal integration at the feature level. Classification algorithms and modern boosting models were used to detect the disease. In addition, the anomaly detection algorithm proved highly effective in distinguishing Parkinson's disease patients from healthy individuals.

The research and the results indicate the potential of combining mixed reality and machine learning technologies in medical diagnostics, while highlighting the technical challenges and the need for further improvements. The work is an important contribution to the development of engineering aimed at early diagnosis and care of patients with neurodegenerative diseases.

#### **Funding:**

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## Mystery molecules under the magnifying glass of scientists – selected experimental techniques for studying amyloids

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Amyloids are highly ordered protein or peptides aggregates, typically forming fibrillar structures and defined by a characteristic cross- $\beta$  architecture. Their formation, both in vitro and in vivo, follows a complex, multistep mechanism that remains incompletely understood. Protein aggregation plays a crucial role in the pathogenesis of numerous neurodegenerative diseases, such as Alzheimer's and Parkinson's disease, but may also serve physiological functions, for instance in bacterial biofilms or gene expression regulation. To elucidate the mechanisms underlying aggregation and to characterize intermediate and final aggregate species, a variety of experimental techniques is employed.

The presentation will provide an overview of selected methods commonly used in amyloid research, including:

a) Fourier-Transform InfraRed (FTIR) and Circular Dichroism (CD) spectroscopies – used to analyze the secondary structure of proteins and peptides;

b) fluorescence assays with Thioflavin T (ThT) – applied to monitor aggregation kinetics;

c) Atomic Force Microscopy (AFM) and Transmission Electron Microscopy (TEM) – used to assess the morphology of formed aggregates;

d) Congo Red (CR) staining – employed to confirm the presence of amyloid-specific structures.

The limitations of individual techniques will also be addressed, along with the importance of their complementary use to obtain a reliable and comprehensive understanding of protein aggregation. The overview will be supplemented by a discussion of cross-seeding interactions occurring between different types of amyloidogenic proteins, which can significantly influence the course and nature of aggregate formation.

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[1] J. A. J. Housmans. G. Wu, J. Schymkowitz, F. Rousseau, A guide to studying protein aggregation, The FEBS journal, 290(3), 554–583, 2023.

[2] S. A. Bondarev, K. S. Antonets, A. V. Kajava, A. A. Nizhnikov, G. A. Zhouravleva, Protein Co-Aggregation Related to Amyloids: Methods of Investigation, Diversity, and Classification, International journal of molecular sciences, 19(8), 2292, 2018.

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[4] M. R. Nilsson, Techniques to study amyloid fibril formation in vitro. Methods, 34(1), 151–160, 2004.

### **Recent advances in protein function prediction**

#### Patryk Jarnot<sup>1</sup>

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Protein function prediction plays a pivotal role in understanding biological mechanisms and improving therapeutic methods. Proteins participate in an array of cell tasks, including enzymatic reactions, signal transduction, structural support, and molecular transport. The ability to predict protein functions not only accelerates discoveries in basic biology but also opens new avenues for medical and biotechnological advancements, such as drug design and disease diagnosis.

In this lecture, we will explore the most recent computational methods for predicting protein functions, highlighting advancements, and remained challenges in the field. We will compare new machine learning techniques to traditional sequence-based approaches. The lecture covers structure-based and network-based strategies, emphasizing their applications and limitations. Additionally, we will discuss the integration of external datasets to improve prediction accuracy. By providing a comprehensive overview, this lecture provides advice on selecting appropriate tools and inspires innovation in methodologies for predicting protein function.

## Signatures of mutational processes in cancer: methods and mechanisms

#### Damian Wójtowicz<sup>1</sup>

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Cancer genomes accumulate a large number of somatic mutations resulting from stochastic errors in DNA processing, naturally occurring DNA damage, replication errors, dysregulation of DNA repair mechanisms, and carcinogenic exposures. These mutagenic processes often produce characteristic mutational patterns called mutational signatures. Identifying and analyzing such patterns can provide essential information on mutational processes underlying cancer development and can have potential implications for understanding cancer etiology, prevention, and therapy. Mathematical and computational tools are indispensable in extracting patterns buried within cancer genomes. I will present computational approaches for studying mutagenic processes and their associations with mutagens and cellular processes through the lens of mutational signatures.

### Trust no one, part I: If it's a reference database it's safe to use, right?

#### Jakub W. Wojciechowski1

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A vast majority of protein sequences available in publicly available databases are derived from genomic data using computational pipelines. Currently over 60% Uniprot records are predicted sequences lacking evidence at protein, transcript, or homology levels. Furthermore, an ever increasing number of genomes, used as an input for such pipelines, originates from metagenomic samples, containing diverse and poorly characterized microorganisms. Assembling such complex data often results in genomic contigs of lower completeness and higher contamination. Considering that the majority of newly characterized genomes comes from metagenomic data, an increasing fraction of sequences are susceptible to errors resulting from contamination, assembly errors, or missing stop codons. These superficial sequences are then incorporated into reference databases undermining the credibility of such resources and affecting biology, medicine and biotechnology. Strikingly, despite this growing threat to the integrity of crucial biological resources, there is little research aiming to address, or even determine the scale of the problem.

## Trust no one, part II: Red flags of your relationship with AlphaFold

#### Alicja Wojciechowska1

#### <sup>1</sup>Department of Biomedical Engineering, Faculty of Fundamental Problems of Technology, Wroclaw University of Science and Technology

AlphaFold's reliance on the homology information and abundance of protein structures gave it the deserved state-of-the-art place in protein structure prediction. This reliance is no problem in the case of commonly studied proteins, but in the case of understudied proteins, it may be. For such proteins, homology information can be tricky, and the low abundance of solved structures additionally harnesses AlphaFold modelling. Here, we will discuss scenarios when AlphaFold struggles to correctly model protein structure. The problematic examples include homologous proteins with different structures, foldswitching proteins and amyloid proteins. Importantly, the diagnosis of such models can be troublesome due to their frequently appearing high-quality scores.

## **POSTER ABSTRACTS**

### Analysing Agent Based Evolutionary Games With Self Creating Strategies

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This project introduces a spatial agent-based simulation model inspired by Evolutionary Game Theory, extended with the capacity for new strategies to emerge dynamically during the simulation process. The simulation operates in a two-dimensional space, where agents—referred to as Individuals—move randomly and only interact with nearby neighbors.

Each Individual possesses a Strategy, which governs energy exchange interactions with other Individuals. An Individual can reproduce asexually upon reaching a specified energy threshold, transferring part of its energy and its Strategy to the offspring. During reproduction, there is a chance that a new Strategy will be generated—a modified version of the parent's strategy, obtained by perturbing its values in the payoff matrix using random numbers from a uniform distribution in the interval [-1, 1]. Each Strategy is uniquely named based on its parent's name and an alphabetical suffix representing its position in the lineage.

Energy is not conserved in the model. Its availability is influenced by an external input function (which may be constant, periodic, or stochastic), energy consumption by Individuals, and gains or losses from interactions. The model supports localized interactions and energy dynamics, leading to complex population and strategic evolution.

We analyze data produced by the model in two primary areas. First, we investigate the evolution of the payoff matrix over time and compare this with classical dynamics in evolutionary theory, aiming to identify whether the model can autonomously reproduce known game-theoretical behaviors. Second, we examine the inheritance of strategies and construct a pseudo-phylogenetic tree to reflect lineage relationships. Our goal is to develop algorithms capable of reconstructing such trees from incomplete information, which could eventually be tested against real biological data.

This model serves as a research framework, intended for iterative expansion with advanced mechanisms and analytical methods.

### Analysis of fibroblast subpopulations in inflammatory skin diseases using scRNA-seq

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The skin is the body's outermost tissue, serving three primary functions: protection, regulation, and sensation. It consists of three main layers: the epidermis, primarily composed of keratinocytes along with a small population of melanocytes, which continually renews itself and protects against mechanical injuries; the dermis, containing fibroblasts, endothelial cells, and extracellular matrix (ECM), providing structural support, thermoregulation, and sensory functions; and the subcutis, a deeper layer of fat and connective tissue acting as an insulator and shock absorber. Skin is continuously surveilled by immune cells, such as lymphocytes, mast cells and macrophages, in order to detect and respond to potential infections. Alterations in skin immune responses and cell composition are a part of the pathogensis of several chronic skin inflammatory diseases such as atopic dermatitis (AD) and psoriasis. These changes can be explored using single-cell RNA sequencing (scRNA-seq), which enables high-resolution profiling of cellular heterogeneity, making it ideal for uncovering rare or specialized cell types within complex tissues.

In this study, publicly available scRNA-seq datasets from skin biopsies were analyzed including epidermis and dermis samples from healthy controls as well as lesional and non-lesional areas of AD and psoriasis patients. The study focused on the heterogeneity of fibroblasts, which are highly diverse mesenchymal cells responsible for collagen production, ECM synthesis, and wound healing. This analysis revealed that a certain fibroblast subpopulation express high levels of SLPI and ELANE. SLPI encodes an inhibitor of neutrophil elastase, playing a protective role against tissue destruction and modulating inflammatory responses. ELANE encodes neutrophil elastase itself, a protease involved in antibacterial defense but capable of damaging host tissues when dysregulated. Typically, neither SLPI nor ELANE are attributed to fibroblast expression, suggesting a potentially novel function for these cells in skin pathophysiology. The datasets were processed using a standardized single-cell analysis pipeline implemented with the Scanpy Python package, incorporating quality control, filtering, normalization, data integration to correct for batch effects, dimensionality reduction, clustering, and cell type annotation. Further analyses included differential gene expression and pathway enrichment to characterize this novel fibroblast subpopulation in healthy, lesional and nonlesional skin samples. The aim of this study is to identify potential surface markers for SLPI and ELANE expressing fibroblasts, enabling their future isolation and functional characterization in vitro, and providing new insights into fibroblast contributions to inflammatory skin diseases.

## Analysis of protein-protein interactions between organisms in the contexts of human-bacteria relationship

Maksymilian Gmur<sup>1,2</sup> Krzysztof Sarapata<sup>1</sup> Jakub Wojciechowski<sup>2</sup> Tomasz Kościółek<sup>2</sup>

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Biochemical processes, signaling pathways, or host-microbe interactions are all mediated by protein-protein interactions (PPIs). Thus, they are important for furthering our understanding of human health and disease. For example, by better understanding interactions between human cells and pathogens or other host-microbiome interactions that play a role in health.

Despite their importance, experimental data on PPIs remain limited. Moreover, experimental methods for identifying PPIs are often time-consuming, costly, and technically challenging, which hinders the large-scale discovery of novel interactions. Those issues were addressed with recent advancements in computational power and machine learning models, which offer more data-efficient strategies for the analysis of PPIs through prediction.

However, significant challenges remain. Most available datasets limit the capabilities of models by presenting mainly intra-species PPIs and a scarcity of experimentally determined negative interactions. These issues create the need for data-generating strategies, which can lead to problems with data leakage between train and test datasets, or with false-negative interactions in train datasets. In cases with ML purposes, where high-quality data is required, those problems can significantly reduce predictive power, especially in inter-species PPIs context. This study addresses these challenges by constructing and analyzing a curated dataset of experimentally verified PPIs between human proteins and bacterial pathogen proteins. In addition to serving as training data for ML models, this dataset is analyzed to extract biologically relevant features, including evolutionary homology, types of methods used in determining the nature of interaction, taxonomic relationships of pathogens and protein sequence length. These insights aim to improve the knowledge of existing data on this type of interaction.

Another key focus of this study is also the generation of negative interaction samples-a difficult task in cross-species PPI research, where the absence of interaction is rarely confirmed. This study investigates multiple strategies for deriving negative samples from positive interaction data, while carefully addressing the risks of introducing redundancy or false negatives into the dataset.

Ultimately, this work highlights existing limitations in PPI datasets and proposes practical steps toward improving data quality and structure, with the goal of advancing machine learning methods for inter-species PPI prediction. It also outlines directions for future data collection and curation to support robust computational modeling in this field.

### A Natural Biomaterial Modified with a Synthetic Polymer for Ophthalmic Applications: The Potential of Decellularized Parsley Root

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In recent years, there has been growing interest in nature-inspired biomaterials that can be applied in ocular tissue engineering. The aim of this study was to evaluate the potential of decellularized parsley root as a biocompatible scaffold for corneal regeneration, reinforced with polyvinyl alcohol (PVA).

Due to its porosity and microstructural similarity to human corneal tissue, the plant-based material was subjected to a decellularization process using mild reagents (L-ascorbic acid, NaCl, CaCl<sub>2</sub>), enabling effective removal of cellular components while preserving the integrity of structural elements. The resulting matrix was impregnated with PVA, a synthetic polymer that improved the scaffold's physicochemical stability and mechanical properties.

The material was characterized using scanning electron microscopy (SEM), thermogravimetric analysis (TG), and in vitro degradation tests in media simulating natural physiological environments: phosphate-buffered saline (PBS), simulated body fluid (SBF), and simulated tear fluid (STF). SEM analysis revealed a uniform, porous structure. TG confirmed thermal stability up to approximately 90°C. Degradation studies demonstrated a controlled mass loss and no significant changes in pH, indicating a mild degradation profile and good biocompatibility.

The developed biomaterial combines the advantages of the natural microarchitecture of parsley root with the functional properties of a synthetic polymer, making it a promising candidate for further research in the field of tissue engineering.

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## Assessment of paroxysmal sympathetic hyperactivity risk in TBI patients using deep canonical correlation analysis

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**Background:** Paroxysmal Sympathetic Hyperactivity (PSH) is a clinical syndrome manifested by heightened autonomous nervous system (ANS) activity caused by traumatic brain injury (TBI). Delayed diagnosis of PSH may result in longer hospital stay, yet early diagnosis remains a challenging task. PSH risk may reflect in desynchronization between ANS and cerebral hemodynamics. Deep Canonical Correlation Analysis (DCCA) is a multivariate method used to examine relationships between two sets of variables.

**The aim:** Early detection of PSH using DCCA applied to ANS metrics—specifically, heart rate variability in the low-frequency range (LF) and heart rate (HR)—and cerebral hemodynamics—intracranial pressure (ICP) and pressure reactivity index (PRx).

**Materials and methods:** We retrospectively analyzed first 24 hours of ICP and arterial blood pressure signals from 52 patients with severe TBI. Patients were grouped into two cohorts: 17 identified as likely to have PSH and 35 considered unlikely, based on the Clinical PSH Assessment Measure. DCCA was performed on pairs of signals and five canonical components were analyzed. The study was approved by the Bioethics Committee of the Wroclaw Medical University (KB-133/2023) and supported by the National Science Centre, Poland (UMO-2022/47/D/ST7/00229).

**Results:** The first five canonical correlations were higher in the no PSH/PSH group: for HR vs ICP 1.00/0.76, 0.94/0.52, 0.86/0.39, 0.57/0.18, 0.01/0.04, for HR vs PRx 0.98/0.85, 0.93/0.77, 0.90/0.71, 0.39/0.32, 0.18/0.02, for LF vs ICP 0.99/0.94, 0.99/0.83, 0.67/0.72, 0.45/0.24, 0.12/0.17, and for LF vs PRx 1.00/0.82, 0.85/0.73, 0.76/0.36, 0.66/0.19, 0.16/0.08.

**Conclusions:** DCCA revealed possible desynchronization between ANS and cerebral hemodynamic metrics, therefore it may effectively differentiate between patients at risk of PSH from those not at risk. To confirm those findings, the study should be repeated on a larger group of patients.

### ATP7B Protein - Bioinformatic Analysis of the Copper -Transporting Protein

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Mutations in the ATP7B gene can lead to Wilson's disease, a rare genetic disorder characterized by toxic accumulation of copper in various tissues, particularly the liver, brain, and kidneys. Clinical manifestations are highly diverse, including hepatic dysfunction, neuropsychiatric symptoms, movement disorders, and psychiatric disorders. Early diagnosis and intervention are crucial for the prevention of irreversible organ damage.

This project contains a comprehensive bioinformatic analysis of the ATP7B gene and its protein product. The functional domain analysis was conducted and allowed to identify conserved regions, such as Heavy Metal Associated (HMA) domains and ATP-binding motifs, critical for copper ion transport across cellular membranes. Homology studies revealed a strong evolutionary conservation of ATP7B among mammals, highlighting its fundamental role in maintaining copper homeostasis. Gene Ontology enrichment analysis further confirmed ATP7B's involvement in processes like copper ion transport and intracellular copper regulation.

These findings highlight how bioinformatic approaches can help explain the mechanisms underlying rare genetic diseases and support the development of targeted therapeutic strategies.

## Automation of the stroke volume calculation in a preclinical approach using an animal model

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Nowadays, data obtained by means of various imaging techniques, such as MRI, CT, USG and others, enables a broad range of in-depth biomedical investigations. As this data becomes increasingly complex, there is a growing demand for advanced bioinformatic tools to perform analysis appropriate to the research questions posed. Much practically important knowledge can be gained from preclinical studies of pathological brain lesions in animal models, performed using magnetic resonance imaging. However, working with such images is difficult and time-consuming, as classic methods of biomedical image analysis often have problems with extraction of lesion-affected brains from raw images, e.g. where the surface of brain is flooded with blood. Regions of interest (areas of pathological changes) often also need to be extracted from the image manually. At the same time, most of the currently available tools and pipelines are created to study the human brain and cannot be used to process and analyze MRI images of other model animals' brains. The goal of our project is to create a pipeline able to (1) accurately extract rat brain from the raw MRI images, and (2) generate a precise mask of a stroke region, which is necessary to determine the location and volume of the stroke, as well as to identify anatomical structures affected by the lesion.

Our data consists of high-resolution T2 MRI scans of rat brains stored in NIFTI format, providing detailed information about the structure of brains under study. We gratefully acknowledge Dr. Bartosz Pomierny for providing the dataset used in this study. The pipeline we are developing is based on Python programming language and Sammba-MRI, a package integrating tools like FSL, AFNI, ANTs, and RATS. Image preprocessing includes data quality control, bias field correction, brain extraction, and template-based registration. We create three optimized brain masks for different analytical needs: a high-precision mask for final volumetric measurements, a rapid geometric approximation for preprocessing, and a conservatively dilated safety-net mask to prevent tissue exclusion and apply the most precise one to extract tissue-specific voxels for downstream analysis. Finally, our pipeline is expected to ensure the standardized and robust processing for rat brain segmentation and the assessment of the stroke area, providing the information crucial for a better understanding of pathological processes affecting the brain.

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## Bioinformatics analysis of the impact of the gut-brain axis on neurodegenerative diseases

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The onset of neurodegenerative processes can be initiated by the interaction between protein products of the gut microbiota and the human body. Gut bacteria produce amyloid proteins which, due to their structured  $\beta$ -sheet conformation, have the ability to aggregate into amyloid deposits. Through the circulatory system, the blood-brain barrier, or the vagus nerve, these proteins can reach the central nervous system. There, they initiate aggregation seeds, disrupting the function of the brain and nerve fibers by promoting the development of neurodegenerative diseases such as Alzheimer's disease, Parkinson's disease, multiple sclerosis, and amyotrophic lateral sclerosis. Analysis of the gut microbiota composition may play a key role in developing early diagnostic methods and assessing the risk of neurodegenerative diseases. Different bacterial species produce distinct metabolites, and metagenomic studies indicate that enrichment or deficiency of specific taxa is associated with the development of these disorders. Therefore, the microbiome composition represents a promising risk marker and a potential target for personalized therapy aimed at modulating the microbiota. In the presented analysis, bacterial proteins from the human gut microbiota capable of aggregating into amyloid structures were identified. The sequences of these proteins were assigned to the corresponding taxa and linked to specific neurodegenerative diseases. Data on amyloidogenic sequences were obtained from the AmyLoad database after prior curation, while information on bacterial species and genera associated with neurodegeneration was sourced from the Human Gut Microbiome Atlas, GMrepo, and Disbiome databases. The proteomes of the relevant species were retrieved from UniProt. By comparing the protein sequences of the proteomes with information from AmyLoad, potentially amyloidogenic bacterial proteins were identified. Their structure was then analyzed using the ESM Metagenomic Atlas tool, which allowed the localization of aggregation-prone fragments and the refinement of the potential risk assessment for the initiation of amyloidogenic processes. This analysis highlights the potential impact of gut microbiota-derived amyloid proteins on the development of neurodegenerative diseases and underscore the importance of further research into microbiome-targeted prevention and therapeutic strategies.

### Comparative Analysis of Transfer Entropy and Conditional Joint Transfer Entropy in Assessing Cerebral Autoregulation

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**Introduction:** Cerebral Autoregulation (CA) is a dynamic, nonlinear process that maintains cerebral blood flow (CBF) in response to changes in mean arterial pressure (MAP). In many studies, CBF is approximated by flow velocity (FV). Traditional approaches, such as Transfer Function Analysis, assume stationarity and linearity, which may not fully capture CA dynamics. To address these limitations, transfer entropy (TE) was proposed as a model-free, information-theoretic method that quantifies directional causality in nonlinear systems. This can be extended using Conditional Joint Transfer Entropy (CJTE), which incorporates a third external variable to modulate the system.

Aim: This study aims to compare the effectiveness of TE and CJTE in detecting causality in CA.

**Materials and Methods:** A total of 24 volunteers (15 females and 9 males, aged  $23 \pm 3$  years) participated in the study (KB-179/2023/N). Non-invasive arterial blood pressure (ABP) was recorded using a photoplethysmograph to derive MAP. FV was measured using transcranial Doppler ultrasound. ETCO2 was controlled using capnography. Measurements were performed during rest and controlled breathing at 6, 10, and 15 bpm. Information flow was assessed in both directions between MAP and FV. In CJTE, ETCO2 was used as a modulating factor. The study was supported by the National Science Centre (UMO-2022/47/D/ST7/00229).

**Results:** Repeated measures ANOVA showed that both TE and CJTE detected a significant effect of breathing rate on information transfer from MAP to FV (TE: p=0.003; CJTE: p=0.007). Posthoc pairwise t-tests with Bonferroni adjustment revealed that only TE detected a significant difference between all breathing rates, while CJTE identified a difference only between rest and 10 bpm. Additionally, TE and CJTE appeared inversely related: as TE increased, CJTE tended to decrease.

**Conclusions:** Our results demonstrate the potential of both entropy-based methods in analyzing the impact of breathing on CA. Further studies with larger cohorts are needed to confirm these findings.

### Comparison and evaluation of similarity network creation methods for TCR repertoire

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Immune repertoires consist of sets of T-cell clonotypes. Analyzing a blood sample provides a snapshot of the T-cell clonotype distribution in a patient. Studying these repertoires provides insights into the inner workings of the immune system. The distribution of T-cell clonotypes can reveal information about the individual's current immune response, potentially indicating whether the immune system is actively combating a challenge and, if so, what that challenge might be. Therefore, it is reasonable to assume that immune repertoire analysis could enable disease detection. This is an exemplary use of a personalized medicine approach in diagnostics, the one that does not rely on potentially misleading symptoms but instead incorporates detailed data on the patient's immune system response.

To make this possible, we must first learn how to decode and correctly interpret the information contained in the immune repertoire. A key indicator of an ongoing immune response is the presence of large groups of highly similar clones or unusually large numbers of unique clones. While it may be tempting to apply clustering algorithms to detect such patterns, the results are often difficult to interpret. As an alternative, immune networks offer a more structured and potentially interpretable way to represent repertoire data.

The goal of this work is to compare different algorithms for constructing immune networks and to identify those that yield the most informative representations for detecting disease-specific patterns. In particular, we examine several variants of approaches for building networks based on distance matrices computed either directly from the sequences or from their numerical vector representations. These variants include the use of different distance functions as well as various methods for generating the numerical embeddings of sequences. We aim to find both disease-specific algorithms and a universal approach that can reliably distinguish between various diseases (or detect the absence of disease).

## Comparison of autologous and allogenic iNKT cells through single cell transcriptomics

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Natural Killer T (NKT) cells combine features of NK cells and T lymphocytes, contributing to both specific and non-specific immune responses. Their therapeutic potential, especially against cancer, is under active investigation.

Autologous CAR-engineered NKT cells targeting GD2 and secreting IL-15 have shown efficacy without dose-limiting toxicity in children with neuroblastoma (2024-NB-News\*). However, challenges like limited cell yield, poor quality, and high production costs restrict the use of autologous CAR-T therapies.

This highlights the need for allogeneic approaches using invariant NKT (iNKT) cells derived from unrelated donors, particularly from induced pluripotent stem cells (iPSCs) or hematopoietic stem and progenitor cells (HSPCs).

This thesis will compare autologous CAR-NKT cells (Heczey et al., Nature Medicine 2020) with allogeneic iNKT cells derived from HSPCs (Li et al., Nature Biotechnology 2024) through single-cell transcriptomics. I will analyze iNKT subsets, metabolic profiles, and potential functional differences relevant for future therapies.

### Decellularized bamboo stem as a biomimetic scaffold for peripheral nerve regeneration

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Peripheral nerve injuries can lead to significant impairments in both sensory and motor functions, and in severe cases, may result in irreversible neurological dysfunction. One of the treatment approaches for such damage involves the use of three-dimensional biomaterial scaffolds developed within the field of tissue engineering. However, designing suitable structures to support nerve regeneration poses multiple challenges, primarily due to the need to meet stringent mechanical, biological, and anatomical requirements. One technique that enables the creation of appropriately structured material is decellularization—a process that removes cells from a given tissue while preserving its natural extracellular matrix architecture.

The aim of this study was to develop and evaluate an implant designed to support peripheral nerve regeneration, based on chemically decellularized bamboo stem. The selection of bamboo was motivated by its internal structure, which closely resembles the architecture of peripheral nerves, making it a promising candidate within the context of biomimetic design. The decellularization process was carried out using milder, less toxic chemical agents, which helped reduce the risk of cytotoxicity and tissue irritation at the implantation site, while also minimizing environmental impact.

The obtained scaffolds were subjected to a comprehensive analysis, including evaluation of their microstructure under conditions simulating the biological environment (in phosphate-buffered saline (PBS) and simulated body fluid (SBF)), physicochemical characterization, and thermal stability testing, which enabled assessment of their suitability for safe sterilization—an essential step prior to any potential clinical application.

The results confirmed that the bamboo-based scaffolds exhibit a structure conducive to peripheral nerve regeneration, both in terms of micro- and macro-architecture. Degradation tests demonstrated that the scaffolds have an appropriate decomposition timeline. Additionally, thermal analysis showed that the implants can be effectively sterilized using low-temperature plasma, confirming their potential safety in clinical settings. The scaffolds were also surface-modified with a polyurethane coating.

In the next phase of research, further studies will be necessary—both on unmodified materials and those with additional surface modifications—to fully evaluate the suitability of bamboo-based implants for peripheral nerve regeneration.

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#### **Deep Phenotyping: Understanding the Details of Disease**

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Deep phenotyping involves the detailed characterization of a patient's observable traits, capturing the diverse types of data they generate throughout their life. This process, often standardized using tools like the Human Phenotype Ontology (HPO), goes beyond traditional clinical descriptions to provide a precise and comprehensive representation of the patient's condition. By establishing a crucial connection with genomics, deep phenotyping enables a more nuanced understanding of the relationship between genetic variations and their phenotypic manifestations. Recent applications of deep phenotyping have demonstrated its power in advancing precision medicine, improving diagnostics, and facilitating the development of novel therapies. Future directions hold the promise of even more transformative applications, further unraveling the complexity of human disease and paving the way for personalized healthcare strategies.

#### Development of a method for protein function prediction

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Proteins are an essential component of every living organism. They are composed of amino acid sequences that determine their structure. Consequent to technological advances, novel functional characteristics associated with specific proteins are constantly being discovered. Due to the growing amount of data, it has become necessary to develop methods for the automatic annotation of protein functions. These annotations are crucial in developing new treatments for diseases, and they improve our understanding of the biological processes in living organisms. A single protein can have more than one gene ontology annotation assigned, therefore, the task falls under the category of hierarchical multi-label classification

In this work, we are testing the performance of classical machine learning methods, such as decision tree, random forest, and k-nearest neighbors, as well as various neural network architectures. We also optimize the hyperparameters of the aforementioned methods using grid search. The dataset used comes from the Critical Assessment of Functional Annotation 5 (CAFA5) challenge, which contains numerous protein sequences and annotations in the form of Gene Ontology (GO) terms. The dataset is already divided into train and test parts. To evaluate the results, we used the maximum F-measure metric, which is based on weighted precision and recall. The score was calculated for each of the three test sets, focusing on all GO categories: Molecular Function, Biological Process, and Cellular Component. Finally, the arithmetic mean of the maximum F-measures was calculated to obtain the overall result.

The experiments showed that deep learning based methods outperformed classical machine learning approaches. However, the results vary between different neural network architectures. Thus, further investigation into the performance of these and other types of neural networks is a promising direction for future research. These results will be further used to develop our own method.

# Effect of Brewing Time on the Antioxidant Potential of Teas and Herbal Infusions

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Antioxidants play a crucial role in neutralizing reactive oxygen species (ROS) and free radicals, which in excess can lead to oxidative stress and damage cellular structures such as membranes, proteins, lipids, and nucleic acids. These harmful compounds are produced both as by-products of mitochondrial metabolism and as a result of inflammation, infection, and stress. The consumption of antioxidants from dietary sources such as vegetables, fruits, teas and herbal infusions is essential for maintaining the body's redox balance.

In our study, we investigated the total antioxidant capacity (TAC) of selected teas and herbal infusions from a single producer, focusing on the effect of brewing time. Using the 2,2'-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) (ABTS) method, we evaluated how different extraction durations affected antioxidant activity. Our results showed that for black, green, and white teas, prolonged brewing significantly increased TAC levels, highlighting the importance of extraction time in maximizing their antioxidant potential. Conversely, rooibos and herbal infusions - including mint, lemon balm, nettle, chamomile, and sage - consistently exhibited low TAC levels regardless of brewing time. We also observed that the antioxidant potential tended to reach a plateau after 7 minutes of brewing time for most teas and herbal infusions.

# From Normal Hematopoiesis to Leukemia: Tracing Malignant Potential Through Single-Cell CNV Patterns

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Leukaemia is a type of blood cancer that starts when blood cells develop abnormally and begin to grow out of control. At the root of this transformation lie genetic and epigenetic alterations that disturb normal haematopoiesis. Increasing evidence suggests that such changes originate already in hematopoietic stem cells (HSCs) — the early, multipotent cells responsible for maintaining and regenerating the blood system. These early changes can remain hidden in stem cells and gradually lead to full-blown leukemia. Single-cell RNA sequencing (scRNA-seq) provides detailed insight into cellular heterogeneity, while integration with copy number variation (CNV) analysis enables the detection of early chromosomal abnormalities associated with leukemic transformation.

In this study, an analysis of bone marrow-derived single-cell transcriptomic datasets from healthy individuals and leukemia patients was performed. After preprocessing using the Seurat R package, data integration and trajectory analysis, the inferCNV tool was applied to infer CNV patterns across individual cells. By integrating CNV profiles with transcriptional states and cell trajectory analysis, distinct leukemic subpopulations with characteristic CNV signatures were identified.

These findings highlight the utility of combining transcriptomic and CNV data at single-cell resolution to detect early signs of malignant transformation which may contribute to the development of more precise, personalized therapies for leukemia.

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## From Pixels to Insights: Challenges and Opportunities of Bioimage Informatics

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Recent decades have seen the development of numerous techniques in light and electron microscopies. Both new ways of constructing optical systems and new types of dyes and labelling techniques for structures at the molecular, cellular and super-cellular levels have enabled the conduct of hundreds of thousands of studies producing vast amounts of imaging data. In order to deal with these data efficiently and process them into state-of-the-art biological knowledge, a new discipline within bioinformatics and computational biology was created in the early 2010s called bioimage informatics [1].

Ongoing efforts in the field aim to address several key challenges. The first family of problems can be described as connected to data handling. Biological imaging data are complex and require large storage space, which makes them difficult to process and share. Commercial softwares of most microscopes export data in proprietary formats often requiring conversion to other formats when accessed using another program. While TIFF is typically considered to be a default safe export choice, there is currently no single standard format for storing biological images. In addition, the information they contain becomes almost impossible to interpret in the absence of a sufficiently detailed description (metadata) [2, 3]. To address these pitfalls, a lot of effort from the contemporary imaging communities, including Open Microscopy Environment (OME), is being put into creating a next-generation file format for large-scale, cloud-enabled use, such as OME-Zarr [4], and spreading the FAIR – findable, accessible, interoperable and reusable – imaging data concept [3]. Another group of problems is related to microscopy image analysis challenges. These may be divided into three main tasks: image restoration, partitioning, and objects quantification. A plethora of tools based on supervised Deep Learning (mainly U-Net Deep Convolutional Network [5] and its derivatives) are being developed to deal with these issues in recent years, although unsupervised approaches, as e.g. μSAM [6], are also emerging.

Overall, bioimage informatics appears to be entering a phase of rapid advancement. Ongoing developments highlight the pressing need for integrative approaches that address both the technical and biological challenges of the field.

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# From prediction to verification: bioinformatic analysis of MCPIP1 as an example of the necessity to integrate computational modeling and experimental research

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The rapid development of bioinformatics methods enables fast prediction of protein structures and functions based on sequence data. However, it still faces fundamental limitations due to the lack of experimental structural information. According to the Protein Data Bank, three-dimensional structures have been experimentally determined for only 235 183 proteins, whereas as many as 1 068 577 protein sequences are known solely through computational models. The large proportion of predicted models significantly limits the reliability of functional predictions for proteins. This study focuses on the analysis of MCPIP1 (Regnase-1), a eukaryotic protein involved in the regulation of immune responses through mRNA degradation, with particular emphasis on the functional role of its PIN domain. The analysis utilized bulk RNA-seq data from murine keratinocytes with silenced ZC3H12A expression, as well as the DALI and AlphaFold tools to investigate homologous domain structures present within the MCPIP1 sequence and their potential functions. MCPIP1 represents a unique case, as its ribonucleolytic activity requires the cooperation of the PIN domain, an intrinsically disordered N-terminus, and a zinc finger motif, while its specificity towards selected transcripts arises from unique structural features, such as an exposed positively charged loop within the catalytic domain. The purification and crystallization of complex, multidomain proteins like MCPIP1 are associated with numerous challenges. Obtaining the full structure of MCPIP1 through experimental methods remains a major challenge, and the currently available fragmentary structures are insufficient to fully validate predictions made through bioinformatic analyses. The results presented in this study highlight that only an integrated approach combining in silico analyses with experimental validation enables the reliable discovery of novel biochemical mechanisms.

# Functional and structural analysis of mutation HFE protein (C282Y) – key to understanding hemochromatosis

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Hemochromatosis is an autosomal recessive genetic disorder that occurs with high prevalence in populations of European origin. Hemochromatosis type 1, which is associated with a mutation in the HFE gene on chromosome 6p22, is an inherited, autosomal recessive disorder of iron metabolism. Excess iron is deposited in a variety of organs leading to their failure, and resulting in serious illnesses including cirrhosis, hepatomas, diabetes, cardiomyopathy, arthritis, and hypogonadotropic hypogonadism. Severe effects of the disease usually do not appear until after decades of progressive iron loading. Mutation C282Y occurs in a highly conserved residue involved in the intramolecular disulfide bridging of MHC class I proteins and could therefore disrupt the structure and function of this protein. The purpose of this analysis was to visualize and understand how the mutation impacts HFE conformation and its functionality. We've created a HMM profile for this protein and its 100 closest sequences from BLAST and focused on this range. Also, AlphaFold 3 and I-Tasser were used to predict structure of mutated protein and those were compared with the experimentally obtained structure. We've observed that simulating the structure of the mutant protein using those tools is problematic. Our study raises important questions about potential treatments for hemochromatosis type 1.

# Functionality and Integration of Information Systems in Polish Medical Facilities: Literature Review and Preliminary Research Findings

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Information systems play a key role in managing medical data, supporting diagnostic processes, treatment and archiving. The aim of the poster is to present a literature review concerning the functionality, integration and challenges related to the use of these systems in Polish medical facilities.

The main types of systems discussed include HIS, RIS, LIS and PACS, along with the challenges related to their integration and interoperability. The benefits of their implementation, such as improved quality of medical services, have been identified, as well as difficulties including high costs and data exchange issues. The offerings of leading system providers in Poland have also been analyzed. The literature emphasizes the importance of full system integration for effective facility management and ensuring continuity of care. Despite the growing interest in digitalization many institutions still struggle with fragmented IT solutions.

The research gathers data from selected facilities to assess the impact of system integration on the quality of healthcare services. The results of this research will expand knowledge about the effectiveness and future of information systems in the Polish healthcare sector.

# Functional Pathway Enrichment of Let-7b-5p Targets in Microglial Response to Ischemic Injury

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Ischemic stroke (IS) is one of the leading causes of mortality and long-term disability worldwide. Microglia, the brain's primary immune cells, play a crucial role in the post-stroke inflammatory response. Under physiological conditions, they maintain homeostasis, but after injury, they shift toward either a pro-inflammatory (M1) or anti-inflammatory (M2) phenotype. One of the key regulators of this polarization is the microRNA let-7b-5p. Increased expression of let-7b-5p has been shown to suppress the M1 phenotype and enhance recovery of neurological function. In contrast, low levels of let-7b-5p are associated with exacerbated inflammation in neuroinflammatory disorders, suggesting its potential as a biomarker of microglial activation. This study aimed to identify let-7b-5p target genes and explore the signaling pathways they affect. Target prediction was performed using the miRDB database (score >80), followed by pathway enrichment analysis via ShinyGO (FDR<0.05, minimum 10 genes). Our analysis revealed that let-7b-5p targets are involved in key pathways such as MAPK (inflammation suppression), PI3K-Akt (microglial survival and M2 phenotype), mTOR (neuroprotective and metabolic functions), and FoxO (oxidative stress response and glial cell survival). These findings indicate that let-7b-5p significantly contributes to post-stroke neuroprotection by modulating inflammation and promoting microglial adaptation.

Overall, let-7b-5p emerges as a promising candidate for both a diagnostic biomarker and a therapeutic target in the context of ischemic stroke and central nervous system inflammation.

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## GastroApp: A Digital Health Platform for Monitoring and Flare Prediction in Inflammatory Bowel Disease

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Inflammatory Bowel Disease (IBD), including Crohn's Disease (CD) and Ulcerative Colitis (UC), requires continuous management due to its chronic, relapsing nature. We introduce GastroApp, a digital health platform designed to enhance the care of IBD patients through real-time data collection and intelligent flare prediction.

The system consists of a mobile application that empowers patients to log symptoms, diet, medication adherence, and overall well-being. Complementing this is a web-based dashboard for healthcare providers, offering a clear overview of each patient's condition and alerts about potential disease flares. The backend enables secure data exchange, real-time synchronization, and the integration of predictive models for risk stratification and clinical decision support.

GastroApp aims to bridge the gap between patients and clinicians by enabling data-driven, personalized, and proactive care. Early feedback indicates high user engagement and the potential to detect flare-ups before they become critical, paving the way for improved outcomes in IBD management.

# Generation of protein structure fragments using a conditional variational autoencoder

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### <sup>1</sup>University of Warsaw

Proteins are macromolecules that, due to their vast array of potential functions, form the basis of life. Those functions are in turn determined by their 3D structures. Experimental methods allow us to determine those structures with remarkable quality. However, some parts of the structure eg. loops display high mobility and do not adopt a fixed position. In order to reliably describe their structure, one would need to consider multiple possible conformations. Here, we present a deep learning based approach that allows us to generate potential structures of such fragments.

Our approach involves using a conditional variational autoencoder where the encoder and decoder are fully-connected neural networks. The model achieves roto-translation invariance by operating on the internal angle representation. The loss function however is computed with the cartesian coordinates reconstructed by iteratively adding subsequent atoms to the chain, which allows us to condition the model on the desired 3D orientation. The model is also conditioned on the amino acid sequence and secondary structure of the generated fragment. This method allows us to generate plausible protein fragments while also controlling their orientation.

# ICCAR (Interactive Cell Camera Analysing Robot) – Presentation of a Robust System Built for Capturing and Analysing Ideal Images of Performed Experiments

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**Introduction:** The growing number of biological experiments in recent years generates large amounts of data, which are the source of the increasingly greater understanding of the human genome. Among this vast amount, images play a key role as they form the core of visualizations in biological experiments. The diversity and volume of data highlight the necessity for automation in the data analysis process.

**Methods:** ICCAR (Interactive Cell Camera Analysing Robot) is a portable black box serving as a darkroom, with a top-mounted camera capturing images of a specially illuminated area where samples are placed. Our device allows users to take identically configured high-quality pictures of examined biological material and save them to a designated storage server or USB driver. Users may later connect to the server to view the collected data via a dedicated desktop application, where they can view collected data or automatically detect, count, and measure the size of the tumors. Application also enables and simplifies access to the obtained results of all conducted experiments and allows for comprehensive management of all of them. ICCAR's main functions like camera operation, image saving, and server connection are made possible by a Raspberry Pi 4 computer. The desktop application was developed using PySide6. Application Programming Interface (API) was created using Python FastApi framework. Algorithms used for image analysis and processing include: lens distortion correction, histogram equalization, image sharpening, semantic segmentation, and segmentation. Image operations were performed using OpenCV and sci-kit image libraries.

**Results:** Thanks to the development of ICCAR, scientists from the Center of Biotechnology at the Silesian University of Technology have access to the dedicated software, which simplifies and automates data collection and archive processes during and after the experiment Conclusion: The development of a device for image recording and analysis enabled acceleration and improvement of all tasks connected with processing and analysing experimental results performed in the "wet" laboratory.

# Identification of New Therapeutic Substances for Ischemic Stroke Treatment Using Artificial Intelligence Methods

## Mikołaj Kikolski<sup>1</sup>

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Ischemic stroke accounts for approximately 90% of all recorded stroke cases and remains one of the leading causes of death and disability worldwide. This research aims to employ artificial intelligence to identify novel therapeutic substances for the treatment of ischemic stroke, with the goal of improving patients' survival rates and post-stroke quality of life. The study specifically targets thymidine phosphorylase 4 (TYMP-4), a protein whose expression dynamically changes during ischemic stroke and has been proposed as a potential therapeutic target.

The proposed framework combines deep learning and reinforcement learning strategies and consists of a generative model based on a transformer neural network (TNN) and a predictive model based on a deep neural network (DNN). These two models are initially trained separately on large molecular databases such as ChEMBL and ZINC20. Subsequently, to generate molecules with desired properties, the networks iteratively refine and train each other using a deep Q-learning approach, producing results of higher quality. The first phase of the generative model's training focuses on producing chemically valid molecules in SMILES notation. In the subsequent phase, where both models are used together, the system is optimized to generate molecules capable of interacting with TYMP-4. Furthermore, the proposed framework is versatile enough to generate molecules optimized for multiple properties, making it a valuable general-purpose tool for proposing targeted therapeutic substances.

# Influence on the accuracy of U-Net based cell segmentation by additional data processing

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Cell segmentation is a critical task in biomedical and biological image analysis, often serving as a precursor to quantitative downstream analysis. Accurate segmentation is essential to avoid skewing results due to false positives (marking nonexistent cells) or false negatives (ignoring actual cells). To this end, various strategies have been developed to improve segmentation performance, with image preprocessing being one of the most impactful approaches.

Image preprocessing involves applying a range of transformations to enhance image quality or emphasize specific features, thereby facilitating more effective segmentation by machine learning models. Among the simplest yet widely used techniques are histogram normalization, which adjusts contrast and brightness distributions, and morphological filters that highlight structural features. These preprocessing outputs can either supplement the original image data as additional input channels or replace it entirely, depending on the architecture and goals of the model. In this study, we systematically evaluated the impact of different preprocessing techniques on segmentation performance. Specifically, we explored the effectiveness of histogram normalization, bandpass filtering, edge detection using convolution kernels (such as Sobel and Laplacian), Gaussian smoothing, and difference of Gaussians (DoG) operators. Each method was integrated into the data pipeline and tested under controlled conditions to assess improvements in segmentation accuracy.

Experiments were conducted using the open-source NuInsSeg dataset, which contains a diverse collection of annotated nuclear images suitable for training and evaluating segmentation models. To quantify performance, we employed widely-used metrics such as the Dice coefficient, Intersection over Union (IoU), precision, and recall. The goal of this comparative analysis is to identify which preprocessing strategies most effectively enhance model performance, with the broader aim of guiding best practices in biomedical image segmentation workflows.

# Interactions of mutational signatures and tumor microenvironment in cancer

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Mutational signatures are distinct patterns of DNA mutations that appear due to various factors such as carcinogens (like smoking or UV light exposure), homologous recombination repair defects, mismatch repair defects, and others. They provide useful information on mutagenesis and cancer development by acting as a biological readout of the tumor's history. The term "tumor microenvironment (TME)" is used to describe various types of cells that are close to the tumor (tumor cells, immune cells, stromal cells and extracellular matrix) and their interactions. The composition of the TME impacts the tumor growth, progression and cancer prognosis.

Understanding both TME and mutational signatures is very important as we seek to create new targeted cancer therapies. Despite this fact, few studies explore the interplay between them. In our work, we analyze the relationships between the tumor microenvironment and mutation counts for each cell type-signature pair across cancer samples. Our aim is to identify co-occurring patterns of interactions that may impact patient prognosis. For example, we found that in patients with lung cancer, cells that express the PD1 marker have a relatively high correlation with a signature called SBS92 (which is a signature connected to smoking) nd SBS3, (which is related to defective homologous recombination-based DNA damage repair). We also noticed that cells with the PDL1 marker have a strong correlation with the SBS2 and SBS13 signatures, which are attributed to the activity of the AID/APOBEC family of cytidine deaminases.

These insights highlight the potential of integrating mutational and microenvironmental data to uncover new therapeutic targets. We believe that our findings could help to expand our understanding of tumor progression and, as a result, support the development of personalized therapies.

## Large scale modelling of Escherichia coli proteomes

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Protein structure prediction has witnessed remarkable advancements in recent years, with the emergence of cutting-edge methods such as AlphaFold, ESMFold, OmegaFold, and Chai-1. These methods have demonstrated unprecedented accuracy in predicting protein structures, revolutionizing the field of structural biology. However, their application at the scale of whole proteomes remains a challenging frontier. This poster aims to present an assessment of the efficacy and reliability of prediction methods when applied to whole proteomes of one of the most studied model organisms, Escherichia coli, as well as its phages. Additionally, it focuses on potential ways of utilising such comprehensive analyses in ways which can aid future researchers.

## Metagenomic bioprospecting of cold-active enzymes

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Cold-active enzymes have attracted significant interest in recent years due to their potential applications across various industries. Among them, pectinases and cellulases are particularly valuable, especially in the food and paper sectors. Their efficiency at low temperatures offers substantial advantages, including energy savings and the ability to perform processes traditionally requiring elevated temperatures under milder conditions. In this study, an algorithm for the extraction of coldactive enzyme genes from metagenomic data is presented, accompanied by laboratory validation of the enzymatic activities. The work began with the extraction of raw metagenomic datasets from environmental samples collected in Svalbard. Predicted genes were subsequently filtered to identify candidates encoding pectinases and cellulases, based on criteria such as sequence length and the presence of full-length open reading frames with defined start and stop codons. Further screening was performed using Hidden Markov Models (HMMs) targeting specific protein domains associated with the desired enzymatic functions. Representative sequences obtained through MMseqs clustering were then subjected to protein structure prediction using AlphaFold, enabling a refined selection of candidates for experimental validation. Selected genes were cloned into pET expression vectors and transformed into bacterial expression strains. Following transformation, plate-based assays were conducted to evaluate enzymatic activity. Positive clones were subjected to protein purification, and their enzymatic kinetics were characterized in detail. Although final results are still pending, preliminary findings indicate the effectiveness of the computational pipeline and experimental strategy for identifying coldactive pectinases and cellulases from metagenomic datasets, highlighting the potential for future industrial applications.

## miRNavigate: Your Gateway to miRNA Biomarker Discovery

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MicroRNAs (miRNAs) are short RNA molecules acting as key post-transcriptional regulators of gene expression, with significant potential in targeted therapies and molecular diagnostics. Changes in miRNA levels are directly linked to the development of many diseases, including cancer, cardiovascular, neurodegenerative, and autoimmune disorders. Exploring miRNA-related molecular mechanisms is crucial for advancing diagnostic and personalized therapeutic strategies.

Currently available tools, while useful, have their limitations, which prevent their use in some analyses. Developing tools and protocols that are friendly to researchers with less experience in bioinformatics, and that allow analysis of data from different experiments is key to better understanding the molecular basis of pathological processes that may be interdependent.

We developed a user-friendly web-based application designed for efficient analysis of RNA-Seq data, specifically focused on identifying differentially expressed miRNAs in physiological and pathological states. Our tool integrates established bioinformatics pipelines - DESeq2 and edgeR, allowing researchers to perform robust differential expression analyses even without advanced knowledge of R programming language or other bioinformatics tools, making it more accessible to biology professionals conducting RNA-Seq experiments.

This application significantly reduces the technical barrier, enabling biological researchers to independently analyze single or comparative datasets to pinpoint deregulated miRNAs and potential biomarkers. While still in improvement, our application allows users to compare results among different datasets as well as different tools. By facilitating straightforward, rapid analysis, our tool supports advancements in understanding disease pathology and accelerates the discovery of clinically relevant miRNA biomarkers in genetic disorders and cancers.

# New Steps – Accessible, 3D-Printed Lower-Limb Prosthesis for Broader Medical Accessibility

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In response to the growing global and national demand for accessible lower-limb prosthetics driven by both chronic diseases and armed conflicts—the New Steps project aims to develop a costeffective, functional prosthesis manufactured with 3D printing technology.

Instead of traditional rigid sockets made of carbon fiber, the project introduces a flexible, adaptable socket made from nylon, inspired by the Socket-less Socket concept by Martin Bionics. This approach allows for dynamic adjustment to changes in limb volume, reducing the need for frequent replacements.

A simplified mechanical knee joint, created using 3D-printed components, offers a significant reduction in production costs while maintaining essential biomechanical functionality.

The project employs digital tools for customized design and additive manufacturing of components. The resulting prototypes are evaluated through a user-centered testing process to ensure practical usability and comfort.

New Steps is a step forward in democratizing access to assistive technologies, combining biomedical engineering with a strong commitment to social equity.

## Nonconventional alternative splicing in Euglenids

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Nuclear genes contain introns that are removed by the spliceosome at the RNA level. Most spliceosomal introns are characterized by conserved GT/AG boundaries, a feature also common in numerous introns present in nuclear genes of euglenids. However, euglenids also possess a distinct class of introns: nonconventional introns. These atypical introns have non-canonical ends, lack a polypyrimidine tract, and form a stable secondary RNA structure that brings the intron ends into proximity. While the aforementioned secondary RNA structure shows some conservation, it is limited primarily to the regions near the intron ends.

If the sequences responsible for efficient intron recognition and excision are poorly conserved, they could arise from random sequences due to chance mutations. Consequently, new introns could emerge within coding sequences, or the boundaries of existing introns could shift, thereby affecting the mRNA sequence and the encoded protein. The latter scenario has been observed in euglenid genomes, where alternative splicing (nonconventional alternative splicing) can generate diverse mRNA molecules due to alternative splicing signals within nonconventional introns or exons. Therefore, the presence of nonconventional introns may promote the evolution of proteins, potentially leading to enhanced adaptation to changing environmental conditions.

Our Goal: This study aims to analyze available euglenid genomes to identify instances of nonconventional alternative splicing and to assess its frequency and impact on the sequences of encoded proteins. We create a dedicated program to find potential sites of nonconventional splicing. Our predictions will be later experimentally validated.

# PHIL (Pipetting Helper Imaging Lid) – one step closer to affordable automation in academic research

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Automated pipetting systems offer the potential to streamline a wide range of experimental procedures in scientific research. However, their relatively high cost and reliance on specialized software often limit their accessibility in academic settings. To address these challenges team consisting of Dettinger, P., Kull, T., Arekatla, G., et al. (2022) developed the PHIL (Pipetting Helper Imaging Lid) pipetting robot. The primary objective of PHIL is to provide researchers with a low-cost, user-friendly solution that maintains the precision typically associated with commercial pipetting systems, while offering greater ease of use.

PHIL leverages 3D printing technology for rapid and customizable production of structural components, significantly reducing manufacturing costs. The robot is built from widely available mechanical parts and features intuitive control software, making it accessible even to users without an engineering background. Its simplified design ensures ease of assembly, operation, and maintenance. PHIL was specifically engineered to minimize human error and enhance reproducibility—critical factors in scientific research. Testing has demonstrated that PHIL achieves high positioning accuracy and liquid dispensing precision comparable to that of traditional manual pipetting. These results confirm its suitability for delivering reliable and reproducible outcomes across various experimental conditions.

As part of the KNSB In Silico project, the applications proposed by the authors will be further evaluated. PHIL significantly enhances the accessibility of pipetting automation in academic laboratories, where financial constraints often hinder the adoption of commercial systems. Key advantages include its low cost, unchallenging construction, microscope compatibility and ease of integration into existing workflows.

Future development of PHIL may involve the incorporation of higher-precision mechanical components to further reduce errors and improve performance. However, such improvements could also result in increased production costs.

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# **POMOKA** - User-friendly software for stratifying long-term survival referenced to age- and sex-matched population data

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Mortality is a primary endpoint in many clinical trials, especially in cardiac surgery, where longterm survival is a crucial marker of treatment efficacy [1-3]. While Kaplan-Meier (K-M) analysis is widely used to estimate survival over time [4], it does not account for key demographic factors such as age and sex. As a result, survival curves for older or high-risk patients may appear poor, even if outcomes are clinically acceptable. This stems from the fact that K-M curves are rarely contextualized against standard life expectancy for age- and sex-matched individuals in the general population. Although national life tables provide such reference data, incorporating them into survival analysis remains complex and is not supported by common statistical tools. To bridge this gap, we developed POMOKA - user-friendly software enabling direct comparison of observed survival with expected populationbased survival, stratified by age and sex.

POMOKA is a software platform designed to automate the generation and analysis of mortality graphs from Kaplan-Meier data integrated from different sources. It organizes the data into two primary sections: imported data and population data, with the latter sourced from the Central Statistical Office system. The imported data section offers user-friendly tools for editing and adjusting the data ranges used for analysis, while the population data section provides a standardized dataset for comparison. The population data is adjusted to closely match the imported data, ensuring that the comparison between healthy and sick individuals is as similar as possible. The software supports diverse statistical tests to allow users to conduct thorough analyses of mortality data from various medical centers.

The application also enables graphical editing of the graphs and the generation of a final report, improving the analysis of mortality data for people involved in medical research. The platform has been tested on various datasets (49,647 patients and over 3 million rows in the measurement table). A pilot implementation is planned in selected cardiac surgery departments in Poland.

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# Psychrophiles Under the Microscope – Molecular Mechanisms of Adaptation of Certain Bacteria to Life in Cold Environments

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Psychrophiles are microorganisms that inhabit cold environments. Thanks to the development of adaptive strategies such as the production of specific proteins or a unique structure of the cell membrane, they are able to survive in extremely low temperatures [1]. Explaining the molecular mechanisms enabling psychrophiles to adapt, grow, and develop under these conditions is one of the key challenges of biotechnology.

One of the adaptation strategies of psychrophilic bacteria to the cold is the production of specialized proteins – including psychrozymes, cold shock proteins (CSP), antifreeze proteins (AFP), cold acclimation proteins (CAP), and ice nucleation proteins (INP). Their distinctive structure, such as a higher number of polar residues on the surface of the molecule and a lower number of bonds maintaining the tertiary and quaternary structures, ensures their activity at low temperatures [2, 3].

An interesting example of psychrophiles adapting to extremely cold environments is the secretion of compatible solutes (CS), extracellular polymeric substances (EPS), and/or biosurfactants [4]. Together with AFP and INP proteins, they act as cryoprotectants. Some of them – for example, trehalose, sucrose, and glycerol (classified as CS) – have found applications in cryopreservation.

Another adaptation strategy of psychrophilic bacteria to cold is an increased content of polyunsaturated, short-chain, branched, or cyclic fatty acids in the composition of the cell membrane [5, 6]. Such a structure helps prevent membrane stiffening at low temperatures, thereby ensuring proper functioning of the microorganism.

Substances secreted by psychrophilic bacteria show enormous biotechnological potential. Their use seems particularly promising for processes occurring under refrigeration conditions – such as lactose-free dairy production or juice clarification – which could not only reduce energy consumption but also operational costs [7].

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# Quadruple bioreactor with redundant data storage and measurement aperture

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**Methods:** The experimental setup comprised a custom-designed quadruple bioreactor system engineered for parallel, comparative studies under rigorously controlled conditions. Each of the four bioreactors functioned autonomously within a unified control framework, enabling simultaneous cultivation experiments with distinct nutrient media while maintaining identical environmental parameters such as temperature, agitation rate, and dissolved oxygen concentration. This configuration facilitated direct comparisons of microbial growth kinetics, metabolic activity, or substrate utilization across varying nutritional environments.

**System Architecture and Redundancy:** Each bioreactor, constructed from borosilicate glass with a 250 ml working volume, was equipped with dedicated measurement and control subsystems to ensure operational independence. pH monitoring employed four isolated pH meters, each with independent power supplies and signal-processing circuits to eliminate cross-interference risks. Similarly, hydrogen concentration was tracked via four hydrogen sensors from DFRobot with segregated data acquisition channels. This hardware redundancy ensured continuous operation even during partial system failures. Temperature management utilized a combination of silicone heating mats positioned beneath each bioreactor and a shared tungsten lamp array mounted above the cultivation platform, providing uniform thermal distribution across all four units. Agitation was implemented via a single orbital shaking platform operating at up to 180 rpm, accommodating all bioreactors simultaneously to ensure consistent hydrodynamic conditions. This configuration induced surface aeration through liquid sloshing rather than submerged impellers, eliminating foam formation risks and the need for torque monitoring. pH dynamics were monitored but not adjusted during experiments, as the system's isolation precluded acid/base supplementation.

**Data Acquisition and Storage:** Sensor data, including pH, hydrogen concentration, temperature, and agitation torque, were sampled at a resolution of 0.2 Hz. Redundant local storage utilized dual industrial-grade flash drives with 64 GB capacity each, configured in a RAID 1 mirroring setup. Simultaneously, real-time data streams were transmitted to a PostgreSQL database on a dedicated server via Ethernet protocol, incorporating role-based access controls and automated checksum validation to ensure integrity.

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## Quantitative Analysis of Endogenous Single-Strand DNA Breaks in Nuclear and Mitochondrial DNA

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Eulermotic cells are expressed daily to numerous factors leading to DNA domage inclus

Eukaryotic cells are exposed daily to numerous factors leading to DNA damage, including single-strand (SSBs) and double-strand breaks (DSBs). Under physiological conditions, SSBs occur much more frequently. While the stability of both nuclear (nDNA) and mitochondrial DNA (mtDNA) has been the subject of increasing research interest, mtDNA has drawn particular attention due to its potential role in aging-related and neurodegenerative disorders.

Our preliminary observations suggest that, per megabase pair, mtDNA accumulates doublestrand breaks more frequently than nDNA. This study proposes a methodological framework for quantitative analysis of endogenous SSBs in various mouse tissues and germ cells using sSTRIDE (SensiTive Recognition of Individual DNA Ends), a high-resolution imaging approach capable of detecting individual DNA breaks. By employing sSTRIDE, fluorescence confocal microscopy, and image-based quantification, it is possible to determine SSB levels and calculate mtDNA-to-nDNA damage ratios across tissue types.

This approach can help uncover tissue-specific patterns of nuclear and genome vulnerability and provide a foundation for future research on the role of mitochondrial genome instability in disease and aging.

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# **Reachability graph for Time Petri Nets**

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Time Petri nets are an extension of classical Petri nets that allow modeling of systems with timing constraints. They can be applied in many fields, such as real-time systems engineering, healthcare workflow modeling, analysis of time-dependent biological processes, and drug development. Challenge in modeling such systems lies in understanding all the possible states such a system can reach over time, especially with some strict timing conditions. However, such an analysis often leads to the state space explosion problem, where the number of possible system configurations grow exponentially with the number of places, transitions and timing constraints. This often makes traditional exhaustive analysis infeasible.

To address this, we can use reachability graphs, which represent all reachable states and transitions between them, enriched with timing information. These graphs are a powerful tool for analyzing complex system behaviors, enabling verification of safety properties, detection of deadlocks, identification of unreachable or unstable states, and validation of time-critical constraints. They support not only the verification of correctness, but also deeper system insights, e.g., identifying unintended delays or unreachable states in a time-dependent model of a signaling pathway.

In this project, I contributed to the development of Holmes, a tool created at Poznan University of Technology to analyze Petri nets. Holmes is designed to aid researchers using Petri net models, offering features for modeling and simulating various types of processes. As part of this tool, algorithms were implemented to generate the Petri Net time reachability graph based on the ideas described in the literature. The implementation focuses not only on generating the graph, but also on providing an interactive visualization to better explore the system's behavior. By enabling the generation of such graphs, this feature allows more advanced analysis of systems where timing constraints are critical. The motivation behind the work was the lack of accessible and extensible tools for formal analysis of time-dependent models in bioinformatics and biomedical engineering. Modeling biological processes, such as gene regulation, signal transduction or pharmacokinetics requires explicit treatment of time and concurrency, making traditional approaches insufficient.

# Refactoring and generalization of mathematical modeling code repository: example of social reinforcement learning in IntelliCages

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Creating novel data analysis frameworks for computational biology requires developing formal notation and writing its programmatic implementation. As mathematical concepts build up and domain knowledge expands, these changes must be reflected in code repository. However, many such repositories start as scripts for one-time data analysis and thus lack the initial phase of software architecture and ontology building, making them difficult to scale. Another challenge involves generalizing existing frameworks beyond their original scope. In some cases, similar analytical principles can be applied to datasets of various structure, created with different data collection methods (e.g. custom or commercial laboratory equipment) or data representations (e.g. continuous vs discrete). Accommodating this diversity with modular structure of data analysis tools encourages reusing existing code in new contexts, leading to directly comparable results. Finally, a desirable characteristic of scientific code frameworks is their clarity and credibility perceived by non-technical end users.

In this poster, I present a case of refactoring medium-sized code repository used for analysing social behavior of mice in cages with built-in automated behavior assessment (IntelliCages). The underlying computational framework combines reinforcement learning models with discrete representation of behavioral events, such as entering cage corners to obtain reward (sucrose), with the ultimate goal of understanding social influence on individual reward-seeking efficiency. The aim of the refactoring was to make the framework compatible with a broader range of study designs. In this context, I want to illustrate how combining object-oriented coding principles, design patterns and unit testing can improve code extensibility. Additionally, I put emphasis on decoupling the stages of data preparation, model fitting and saving the results, which helps track progress of large, error-prone analyses and simplifies generation of publication-ready graphs.

# Scanning Electron Microscopy - Methodology, Sample Preparation, and Imaging

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Scanning Electron Microscopy (SEM) is a microscopic technique that utilizes a focused beam of electrons to image the surface of a sample based on signals generated by secondary and backscattered electrons. This allows for the visualization of the surface topography in high detail, often producing a three-dimensional impression of the sample. This method is characterized by high resolution and considerable depth of field. The samples intended for imaging must exhibit electrical conductivity and be free of surface charge. Non-conductive samples require specific preparation procedures, such as fixation and drying (in the case of biological specimens), followed by the application of a thin conductive coating, typically carbon or gold.

Within the scope of the project, participants became familiar with the construction and operational principles of a SEM. Samples were carefully prepared for imaging, and a series of micrographs was obtained. The imaged objects included: a carbon-coated fragment of a butterfly wing from the species Aglais io, gold-coated calcium carbonate crystals, carbon-coated erythrocytes fixed in glutaraldehyde on ITO coated PET, cat hair, and a segment of a spider leg. The resulting images will be utilized for educational purposes and for the promotion of the technique described. The obtained results may serve as a foundation for further in-depth studies and the preparation of scientific papers.

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# Structural and Functional Analysis of BCL-2 Protein: Impact on Apoptosis Regulation and Lymphoma Therapy

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Many diseases, including cancers, are caused by abnormal protein sequences or structures. A particularly interesting case is the BCL-2 protein, a key regulator of apoptosis, whose overexpression in non-Hodgkin lymphomas leads to the inhibition of natural cell death. The discovery of BCL-2 inhibitors, such as Venetoclax, has opened new possibilities in targeted therapy.

In our project, we conducted a systematic review and bioinformatic analysis of the BCL-2 protein, focusing on its molecular structure and functional role in lymphoma development. Using advanced bioinformatic tools, we analyzed available data regarding the sequence, structure, and interactions of the BCL-2 protein, as well as the mechanism of action of its inhibitors.

The analysis revealed that BCL-2 is characterized by a dominant  $\alpha$ -helical motif with a central hydrophobic pocket, crucial for apoptosis regulation. A particularly interesting observation is the region 130-160, which shows high evolutionary conservation, suggesting its critical role in protein function. Analysis of the BCL-2-Venetoclax complex provided better understanding of the specific mechanism of blocking interactions with proapoptotic proteins.

Our results confirm the effectiveness of Venetoclax as a selective BCL-2 inhibitor, particularly in monotherapy and combination regimens with rituximab. The best therapeutic effects were observed in lymphomas with high BCL-2 expression and t(14;18) translocation. We also identified a key therapeutic challenge: the development of resistance through alternative cell survival pathways. These findings have significant implications for optimizing treatment strategies and overcoming resistance mechanisms in lymphoma therapy.

# Sweeping inconvenient data under the rug and fishing for significance - an introduction to QRPs

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Questionable Research Practices (QRPs) are behaviors that, while not always intentional, undermine the integrity and reliability of scientific research. The National Academies of Science defined QRPs as "actions that violate traditional values of the research enterprise and that may be detrimental to the research process." The most common forms include HARKing (Hypothesizing After Results are Known), cherry-picking, p-hacking, and data fishing. Although the discussion around QRPs began more than 50 years ago, awareness of these practices remains limited, especially among early-career researchers.

We were curious whether this phenomenon appears among students in our faculty (FBBiB UJ). To explore it, we designed a survey study in which participants answered questions about their experiences with various research practices. The results of this study are presented on our poster to highlight key trends in our scientific community. We also prepared a checklist of good research practices to support more reliable and transparent scientific work.

The aim of our poster is to raise consciousness about these methods. The knowledge about QRPs is particularly important in the age of data-driven research - especially for bioinformaticians, as we often work on large datasets which require a different approach than traditional academic practices.

To engage our audience, we prepared two QR codes: one linking to an interactive quiz where participants can test their ability to spot questionable research practices in charts, figures and experimental setups based on real examples. The second one leads to a survey prepared specifically for the conference participants, allowing us to compare results between different scientific communities.

## The Protein Crystallization Oracle - a deep learning framework for protein crystallizability prediction

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Determining protein structures is a crucial step in many fields of research, including biotechnology, molecular biology, and drug discovery. X-ray crystallography remains the most widely used technique for experimental structure determination. However, the process from gene to structure is long, labor-intensive, and involves multiple stages—protein expression, purification, crystallization screening, and diffraction testing—each with a high chance of failure. Accurate prediction of crystallizability can reduce experimental costs and accelerate structural research by informing the selection of promising targets.

In this work, we introduce the Protein Crystallization Oracle, a deep learning framework aimed at predicting the likelihood of crystallization based on the target protein's sequence. We describe the PCO's architecture and some of the challenges we faced during training. We also explore the use of explainable AI methods, such as SHAP (SHapley Additive exPlanations), to demystify the model's predictions. This helps identify which sequence features most influence crystallization outcomes, offering valuable insights that can guide the design of more crystallizable proteins.

# Transfer Learning-Based Comparison of Deep Neural Network Architectures for Chest X-ray Classification

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This study aims to compare the performance of selected deep neural network architectures in the task of chest X-ray image classification using a transfer learning approach. Various pre-trained models were adapted to a binary classification problem: healthy vs. diseased lungs. A two-phase training process was employed, consisting of feature extraction and subsequent fine-tuning. Models were evaluated in terms of accuracy, training time, and computational demands. The findings offer practical guidance for selecting appropriate architectures based on the constraints and needs of clinical or technological applications.

# Using Machine Learning to find a novel cytoarchitectonic area in congenitally blind humans

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Fetal maturation is indicated with rapid neurogenesis and hierarchical patterning of the visual cortex (VC). Even so, developmental aburation of visual stimuli e.g. creation of cataracts, can irreversibly disrupt this program and precipitate lasting structural and functional deficits. Yet, congenitally blind people, perform well in everyday tasks without use of visual system, exhibiting superior performance on non-visual memory and spatial tasks, underpinned by extensive cross-modal reorganization of occipital regions. Here, we ask whether a cytoarchitectonically defined hybrid cortex (HC) - originally identified in enucleated macaques between Brodmann areas 17 and 18 emerges in the human blind brain, and how intrinsic neurogenic cues interact with cross-modal plasticity.

The aim of the study is to combined high-resolution quantitative MRI (qMRI) and diffusion MRI (dMRI) at 3 T with magnetization-prepared 2 rapid acquisition gradient echo (MP2RAGE) a highly complexed measure method of bias correction to capture a multi-parameter map (R1, R2\*, MTsat, MTV, PD) and diffusion indices (MD, RD, AD, FA) across the entire brain and within visual ROIs (V1–V3) of congenitally blind (n = 21) and age-matched sighted controls (n = 23). All data were preprocessed in FreeSurfer and analyzed via a Python-based pipeline (NumPy, Pandas, NiBabel) to extract voxel-wise metrics of cortical thickness, surface area, curvature, and superficial U-fiber density.

Blind participants displayed a discrete zone within calcarine cortex exhibiting mixed microstructural signatures—thickened cortex, elevated R2\* and MTsat, and diffusion properties intermediate between V1 and V2—consistent with an HC-like phenotype. These findings reveal that intrinsic neurogenic patterning can manifest even in the absence of retinal input, and that cross-modal plasticity co-opts developing cortical scaffolds to support high-order cognition. Our results bridge macaque and human neuroanatomy, offering new targets for interventions aimed at harnessing neuroplastic potential in blindness and beyond.

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