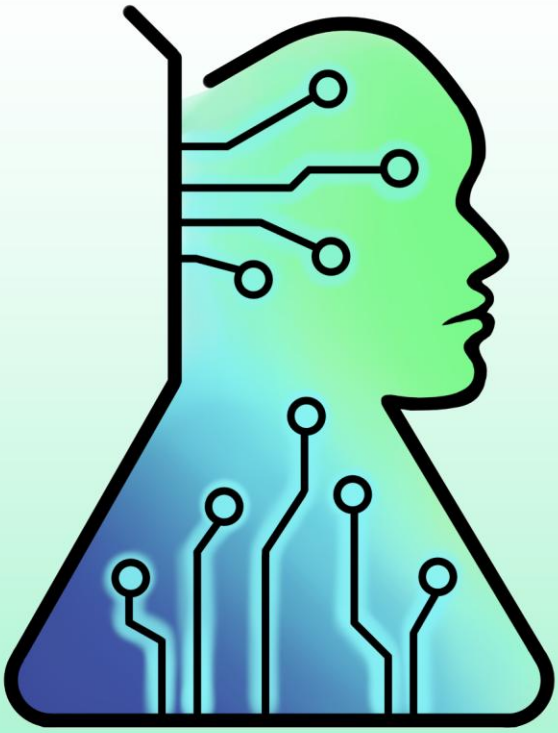
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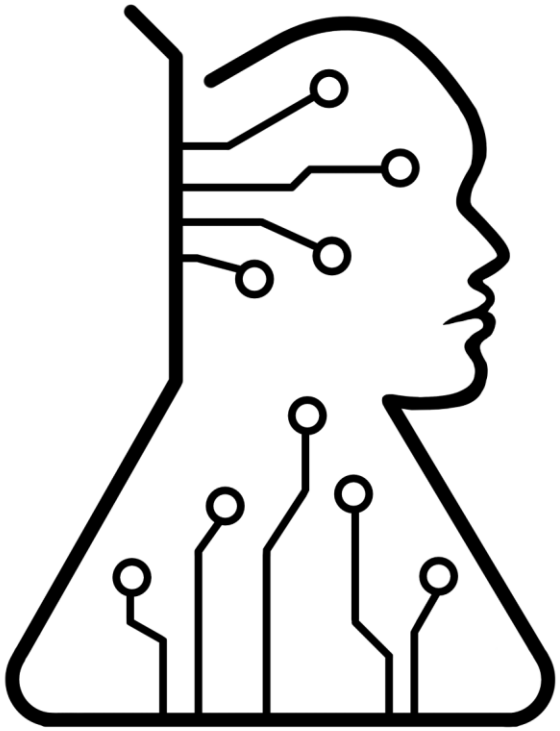
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BOOK OF ABSTRACTS

KONFERENCJA KÓŁ NAUKOWYCH

BioMeeting

PRZESIEKA, MAY 22-24 2026



Coordination and editing
FILIP PIĄTEK

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ADAPTING AN IMC FOUNDATION MODEL FOR PREDICTION OF CLINICAL FEATURES

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Keywords: Imaging Mass Cytometry; deep learning; foundational models; clinical prediction; model interpretability

Imaging Mass Cytometry (IMC) provides spatially resolved measurements of over 40 protein markers in a single tissue section, enabling detailed characterization of tissue architecture and the tumor immune microenvironment. As public IMC resources increasingly include clinical annotations, an important question is whether representations learned by large pretrained models can be transferred to clinically relevant prediction tasks.

We address this question using ImmuVis, a recently introduced foundation model for IMC trained by self-supervised marker reconstruction on 28 cohorts, 24,405 images and 265 markers. We adapt the model for clinical classification by replacing the reconstruction decoder with a hierarchical multiple-instance learning head that aggregates patch-level information into sample-level predictions. We then compare the predictive utility of frozen pretrained embeddings against task-specific fine-tuning on data from 6 IMC panels obtained from 1659 patients from 5 cohorts.

Beyond predictive performance, we investigate interpretability by identifying molecular markers and spatial regions that contribute most strongly to classification decisions, and by assessing whether these patterns are consistent with current biological and medical knowledge. Our study evaluates foundation modeling as a practical starting point for clinically oriented analysis of IMC cohorts and explores when additional fine-tuning is needed for downstream use.

ADVANCING COMPUTATIONAL BIOLOGY WITH DEEP LEARNING FOR NEXT-GENERATION RNA THERAPEUTICS

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Keywords: RNA biology / Deep learning / RNA structure prediction / RNA therapeutics

RNA molecules play central roles in biology and are emerging as powerful therapeutic agents, yet their structural complexity and dynamic behavior remain poorly understood. Recent advances in artificial intelligence have transformed protein structure prediction, but comparable methods for RNA remain underdeveloped due to limited structural data and the complexity of RNA folding and interactions.

My newly created group at the University of Warsaw aims to establish an interdisciplinary research program integrating deep learning with high-throughput experimental RNA biology. The work focuses on three interconnected areas: (i) understanding RNA–small molecule interactions using SELEX-derived datasets and generative AI, (ii) developing AlphaFold for RNA, an RNA-specific deep-learning framework integrating language-model embeddings and experimental probing data for RNA 3D structure prediction, and (iii) designing context-aware therapeutic mRNAs through generative modeling.

The group will generate new computational frameworks that integrate experimental RNA data directly into predictive and generative AI models, enabling improved RNA structure prediction and RNA design.

By combining computational and experimental approaches within a unified framework, this research will advance understanding of RNA structure and function while enabling the development of RNA-targeted therapeutics, RNA-based diagnostics, and next-generation mRNA technologies.

AMELOGENIN – A MODEL BIOMOLECULE FOR INVESTIGATING PROPERTIES AND PATHWAYS OF SELF-ASSEMBLING PROTEINS

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Keywords: amelogenin, aggregation-prone regions, liquid-liquid phase separation, amyloids

Some proteins do not have a well-defined structure and instead contain spatially flexible, intrinsically disordered regions. These regions can drive self-assembly through aggregation-prone sequences, resulting in the formation of structures such as amyloid fibrils, amorphous aggregates, or liquid-like condensates formed via phase separation.

Although it is known that intrinsically disordered proteins can adopt multiple aggregate forms depending on various factors, the underlying mechanisms remain unclear. Amelogenin provides a potential model, as it forms diverse structures depending on isoform length, amino acid composition, and proteolytic processing.

Bioinformatic analysis identified a specific sequence within amelogenin that is likely to govern its self-assembly behavior, while according to the literature, variation in protein and fragment length determines the formation of either amyloid-like, amorphous or small circular aggregates.

These findings contribute to a better understanding of how specific sequence features regulate self-assembly in intrinsically disordered proteins. Investigating the determinants of these pathways may help clarify general principles of protein aggregation and improve our knowledge on aggregation-related health outcomes. Such insights may also support future studies aimed at predicting or modulating aggregation behavior in biological and biomaterial contexts.

Analysis of Difficult Regions in RNA 3D Structure Prediction Based on CASP and RNA-Puzzles

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Keywords: RNA structure prediction, TM-score, non-canonical base pairs, structural topology

Understanding the tertiary structure of RNA is crucial for determining its biological function, yet accurate computational prediction remains challenging. Community-wide competitions such as CASP and RNA-Puzzles provide valuable benchmarks for evaluating prediction methods.

While previous studies have analyzed isolated modelling challenges, the conclusions were insufficient to reduce the disparity between predictions and the real structure. Addressing this gap, our studies focus on identifying recurring patterns in poorly modeled regions and attempting to better understand the sources of prediction errors using benchmark data. We assess prediction accuracy using global similarity measures such as TM-score, examine the role of non-canonical base pairs, and compare structural topologies using tree-based representations.

Our results show that prediction errors tend to cluster in specific structural motifs, particularly in regions rich in non-canonical interactions and complex topologies. The low detection rate across the majority of participants suggests that these motifs represent systematic challenges for current prediction methodologies.

These findings improve our understanding of the limitations of RNA structure prediction methods and can support the development of more accurate algorithms. The combined analysis of tree-based representations, sliding window TM-score, and non-canonical interactions allows for the effective identification of regions that pose a challenge in blind prediction contests.

Analysis Of Gut Microbiome Proteins And Their Interactions

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Keywords: microbiome, gut, proteins, protein–protein interactions (PPI), host-microbiome interactions, secretome

The composition and functions of the human gut microbiome have been linked to a wide range of health conditions, including digestive diseases, neurodegenerative disorders, allergies, and inflammation. The host-microbiome communication happens through various processes, one of which involves microbial secreted proteins that may interact with human proteins. Analyzing and understanding microbiome's secretome would allow us to better understand its functions and contribute to the development of new treatments. In this project we aimed to obtain a dataset of secreted microbial proteins from the human gut microbiome. Therefore we conducted a benchmark of multiple tools for cellular localization prediction. We compared two approaches - direct prediction of protein sublocalization with DeepLocPro and BUSCA, and classification based on combined data regarding the presence of signal peptides and transmembrane regions from SignalP and deep TMHMM. The resulting dataset is an important resource to test for protein-protein interactions with the host. For this purpose we tested the performance of RF2-Lite, but the bottleneck turned out to be the need to generate a high-quality pMSA of cross-species proteins as an input. This work advances current knowledge by providing carefully examined resources for studying microbiome proteins and marking the current possibilities and computational limitations of their analysis.

APTAMER-BASED BIOSENSOR FOR DETECTION OF TNF-ALPHA LEVEL IN SWEAT

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Keywords: TNF-alfa, aptamers, biosensors, IBD

Inflammatory bowel diseases (IBD) are chronic conditions requiring continuous monitoring due to their relapsing nature. Recent advances in wearable biosensing enable non-invasive tracking of biochemical markers, offering new possibilities for patient-centered healthcare.

In this work, we present an aptamer-based electrochemical biosensor designed for integration into a wearable system for real-time monitoring of TNF-α in sweat. TNF-α is a key inflammatory cytokine associated with IBD progression and therapeutic response. Previous studies indicate that sweat TNF-α levels correlate with systemic inflammation and can differentiate between disease states, supporting its potential as a non-invasive biomarker.

Building on this premise, our approach focuses on selective aptamer recognition combined with electrochemical signal transduction in a flexible sensing platform compatible with continuous monitoring applications. The proposed biosensor enables selective and sensitive detection of TNF-α within physiologically relevant concentration ranges observed in inflammatory conditions.

This work contributes to the development of integrated digital health solutions, where wearable biosensors coupled with mobile applications provide continuous insight into patient status. Such systems may improve disease management, allow early detection of exacerbations, and support personalized treatment strategies in IBD.

ASSESSMENT OF EPIGENETIC AGING IN NEUROLOGICAL DISORDERS: COMPARISON BETWEEN CORTICAL AND HORVATH EPIGENETIC CLOCKS

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Keywords: epigenetic clock, epigenetic aging, neurological disorders, Horvath Clock, Cortical Clock

Epigenetic age, estimated from DNA methylation patterns, reflects biological aging beyond chronological time. Its acceleration has been linked to neurological disorders, potentially capturing processes such as neuroinflammation and cellular dysfunction. However, findings remain inconsistent, underscoring the need to investigate epigenetic aging across diverse brain conditions and to compare different epigenetic clocks.
Our motivation was to provide brain tissue-based evidence on epigenetic aging across neurological disorders, including Alzheimer's disease, Parkinson's disease, multiple sclerosis, Down syndrome, and epilepsy. Previous findings remain inconsistent, and studies based on brain tissue are still limited, particularly in epilepsy, where data on epigenetic age are largely lacking. In addition, the Horvath and Cortical Clocks may yield divergent estimates, highlighting the need to systematically compare their performance across neurological conditions.
In Parkinson's disease, Lewy body disease, and Down syndrome, the cortical clock indicated increased epigenetic age compared to controls, whereas temporal lobe epilepsy showed decreased epigenetic age. Results varied depending on the clock used.
Our results extend previous work on epigenetic aging in neurological disorders by jointly analyzing multiple brain diseases and comparing different epigenetic clocks in brain tissue. We show that clock choice can influence biological interpretation, indicating that epigenetic age estimates are not fully interchangeable.

ASSESSMENT OF FOLDAMER PEPTIDES STABILITY VIA CIRCULAR DICHROISM SPECTRA MEASUREMENT

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Keywords: peptides, non-canonical amino acids, secondary structure, α-helix

Circular dichroism (CD) spectroscopy is a commonly used method for studying proteins and other chiral molecules. It detects differences in the absorption of left- and right-circularly polarized light, allowing insight into molecular conformation.[1]

The purpose of this study was to perform a temperature-dependent analysis of the secondary structure of foldamer peptides using CD spectroscopy. The work focused on novel peptide foldamers – synthetic oligomers designed to adopt stable, well-defined, and predictable conformations. The inclusion of non-canonical amino acid residues can improve structural control, resistance to proteolysis, and biological functionality [2].

Two 30-residue foldamers with identical sequences were examined, differing only in the substitution of leucine with cycloleucine in one variant. CD spectra were collected at pH levels of 3.0, 7.2 and 9.0, and thermal stability was evaluated over a temperature range of 4–96°C.

Both foldamers displayed CD spectra typical of α-helical structures, with negative bands around 207 and 222 nm. Only slight variations in signal intensity were observed across the tested pH and temperature conditions, indicating that the secondary structure remained largely intact. These findings suggest a high degree of conformational stability under different environmental conditions, supporting potential applications in areas such as drug delivery systems [2].

[1] S. R Martin, et al. (2008) Methods in cell biology vol. 84. doi: 10.1016/S0091-679X(07)84010-6
[2] M. Szefczyk, et al. (2025) J. Mater. Chem. B 13, doi: 10.1039/D5TB00752F

BACTERIAL PROTEIN TOPOLOGY AS A NOVEL ANTIBIOTIC TARGET

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Keywords: antibiotic resistance, knotted proteins, TrmD, topological proteomics, drug discovery

The persistent rise of antimicrobial resistance constitutes a profound challenge to global public health, exacerbated by a historical reliance on a narrow range of bacterial targets such as DNA replication and protein synthesis. As conventional antibiotics lose efficacy, the focus of pharmacological research must shift toward identifying unique biochemical structures that distinguish bacterial pathogens from their eukaryotic hosts.

This overview examines knotted proteins—rare polypeptides whose backbones form non-trivial topological entanglements—as a viable yet underexplored class of therapeutic targets. While these structures pose significant kinetic challenges during protein folding, their evolutionary conservation across essential bacterial enzymes suggests they provide indispensable structural stability and catalytic precision. The primary finding of this synthesis is that the profound structural divergence between bacterial knotted enzymes, such as TrmD, and their unknotted eukaryotic counterparts, such as Trm5, facilitates the design of highly selective inhibitors. By exploiting these topological disparities, researchers can develop agents that disrupt essential bacterial functions with minimal risk of host toxicity. This topological approach represents a paradigm shift in drug discovery, offering a robust strategy to overcome "evolvability" in resistant strains by targeting structurally constrained, essential protein folds.

BIOINFORMATICS IN CONTEMPORARY MRNA VACCINE ENGINEERING

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Keywords: mRNA vaccines, artificial intelligence, bioinformatics, lipid nanoparticles

Messenger RNA (mRNA) vaccines are an alternative to traditional vaccines by utilizing the host's own cells to produce antigens. Rapidly developed during the COVID-19 pandemic, they have demonstrated high efficacy and a strong safety profile. Their high programmability combined with the potential for fast and low-cost manufacturing makes them a promising tool for personalized medicine. In this poster, we aim to explore the prospective application of artificial intelligence and bioinformatic tools in optimisation of mRNA vaccine design process. The main methods discussed include, but are not limited to, NetMHCpan-4.2 for epitope identification, LinearDesign for mRNA sequence design and machine learning models for predicting key characteristics of lipid nanoparticles (LNPs). These computational methods, along with emerging biotechnological advancements, pave the way for a future where mRNA vaccines are the cornerstone of personalized medicine.

BRAIN ATLAS REGISTRATION ACCURACY IN STROKE: REVIEW OF IMPLICATIONS FOR PARCELLATION CHOICE

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Keywords: stroke, brain parcellation, functional connectivity, review

Resting-state functional connectivity (FC) analysis relies on brain parcellation atlases to define network nodes. Anatomical atlases (e.g., AAL) use structural landmarks, while functional atlases (e.g., Schaefer) derive from connectivity gradients. In stroke, structural lesions disrupt brain anatomy, yet their impact on different atlas modalities remains insufficiently characterized.

Standard spatial normalization pipelines (ANTs, SPM) can produce inaccuracies in stroke imaging, as hypointense lesions induce warping artifacts that displace atlas boundaries. Although lesion masking mitigates errors, research comparing anatomical versus functional parcellations' topological robustness remains scarce.
Since functional boundaries reflect connectivity patterns rather than anatomical landmarks, they may offer greater resilience to structural deformations.
Literature reveals anatomical parcellations are frequently displaced in perilesional territories due to registration errors. While lesion masking partially addresses this, direct comparisons of AAL versus Schaefer frameworks in stroke cohorts are notably absent.

Consequently, stroke connectomics findings may be influenced by atlas choice, particularly when lesion-atlas interactions are not explicitly addressed. Optimizing atlas selection is vital for the development of reliable biomarkers for patient recovery. This review underscores that validating functional atlases is a necessary step toward more accurate and reproducible clinical brain research.

COMPARISON OF SKELETONIZATION METHODS FOR VASCULAR STRUCTURES

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Keywords: skeletonization, image analysis, topology, vascular imaging

Accurate skeletonization of vascular structures is essential for quantitative medical image analysis, enabling reduction of vessels to one-pixel-wide centerlines while preserving topology. Reliable centerline extraction is particularly important in morphometric and hemodynamic studies of cerebral vasculature.

Initial qualitative assessment identified the Zhang–Suen and Lee algorithms as providing smoother and more continuous vessel representations than alternative methods. Binary masks from ICA (n = 526) and DCA (n = 134) datasets were preprocessed and pruned to remove short branches and reduce spurious bifurcations. Evaluation included the Jaccard index, modified Walsh metrics, and normalized branch-point counts.

Both algorithms achieved similar global accuracy; however, the Lee method consistently generated fewer artificial branch points, producing cleaner vascular topologies.

The results demonstrate that branch-point normalization and pruning are essential for reliable assessment of skeletonization methods and may improve downstream vascular morphology and flow analyses.

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COOL APLICATION FOR MIRNA NETWORK AND PREDICTION – VERSION: MAROON

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Keywords: miRNA, enrichment analysis,

MicroRNAs (miRNAs) are key post-transcriptional regulators that influence gene expression and play an important role in diverse biological processes and diseases. Computational analysis of miRNA–gene interactions and their associated pathways has become essential for interpreting high-throughput biological data.

Despite the availability of multiple enrichment tools, there is a lack of lightweight, user-friendly applications specifically focused on miRNA–gene–pathway relationships without domain-specific bias. To address this gap, we developed CATNAP, a bioinformatics application for miRNA enrichment analysis implemented in the R programming language using the Shiny framework. The tool enables users to analyze genes regulated by selected miRNAs with customizable parameters, including prediction score thresholds and pathway size. Data are retrieved from a locally stored miRDB database and processed using established packages such as clusterProfiler and KEGGREST, with results presented as interactive tables and visualizations.

CATNAP provides a fast and focused approach to identifying biologically relevant pathways associated with miRNAs, offering results comparable to existing platforms while maintaining simplicity and flexibility

By emphasizing usability and specificity, the application supports efficient exploratory analysis and may facilitate broader adoption of miRNA-based functional studies in bioinformatics research.

CORONARY VESSEL SEGMENTATION FROM ANGIOGRAPHY

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Advances in computational technologies have significantly improved medical diagnostics by enabling efficient processing of complex data. This progress has facilitated the development of deep learning methods for coronary vessel analysis in angiographic images.

Three architectures (U-Net, Attention U-Net, and two-branch U-Net) were evaluated for coronary vessel segmentation. Experiments were conducted on the ICA dataset (616 images) and the DCA1 dataset (134 images), with and without data augmentation. Focal loss was applied to address class imbalance. Training was performed on ICA and on a combined ICA+DCA1 set. Generalization was assessed by testing ICA-trained models on DCA1. Performance was measured using Dice, clDice, IoU, precision, and recall with K-fold cross-validation. Additionally, preliminary attempts were made to extend the approach to multiclass segmentation using the ARCADE dataset.

Based on K-fold cross-validation and evaluation on the independent DCA1 dataset, the classical U-Net with data augmentation proved to be the most effective model overall. Attention U-Net and two-branch U-Net also achieved good and stable results. Data augmentation improved training and reduced overfitting.

Accurate vessel segmentation supports analysis of vascular structure and improves diagnostic workflows through automation and objectivity.

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De Novo Ligand Generation and Evaluation Using Docking – an Automated Approach

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Keywords: de novo drug design, molecular docking, SMINA, REINVENT

The vastness of chemical space makes purely experimental drug discovery highly inefficient. Computational approaches - particularly de novo molecular design enhanced by recent advances in deep learning - address this by generating novel ligands with specific target properties. However, the rapid and reliable evaluation of these de novo ligands remains challenging due to a lack of benchmark data. Because a promising drug candidate must bind to its receptor with sufficient affinity, a validation framework for generated ligands could incorporate molecular docking.

A major limitation of conventional docking is its reliance on empirical scoring functions. These functions often struggle to accurately predict binding affinity, as their performance can vary significantly across different test sets. For newly designed ligands that diverge from known chemical spaces, a robust, system-independent scoring approach is critical. This suggests that a more physically grounded estimation of interaction energy is required to reliably assess de novo molecules.

Overall, the objective of this work is to build an automated workflow that facilitates the comparison of different scoring functions used in docking simulations. Integrating generative ligand design with molecular docking that utilizes reliable scoring methods will ultimately enhance the identification of promising drug candidates and advance future developments in structure-based drug design.

Development of a Modular Ex Vivo Organ Perfusion Platform for Physiological Monitoring

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Keywords: ex vivo perfusion, organ preservation, normothermic perfusion, physiological monitoring, biomedical engineering, open-source platform.

Thousands of transplantable organs are discarded annually because static cold storage cannot maintain viability or provide real-time functional assessment during transport. Normothermic machine perfusion (NMP) addresses this by maintaining tissue under warm, oxygenated flow. Normothermic ex vivo perfusion of porcine organs has become a critical validation step in xenotransplantation workflows following recent landmark pig-to-human kidney and heart transplants procedures.

Published open-source NMP systems still require budgets of approximately $48,000-66,000 budgets and clinical-grade blood products. This work presents our approach to an NMP-inspired system: a student-built prototype developed by SKN SzczURek at the University of Rzeszów to reproduce selected features of normothermic perfusion using flexible manufacturing, modular construction, connectivity, telemetry, and practical affordance. The experimental scope is limited to ex vivo perfusion physiology on post-slaughter biological material and prototype validation; no live-animal experiments are included.

The main outcome is a connected, modular prototype concept that provides a feasible educational baseline for controlled ex vivo perfusion studies outside clinical NMP infrastructure.By releasing hardware, firmware, and software as open-source materials, our device may help academic groups test perfusion protocols, evaluate haemoglobin-based oxygen carriers (HBOCs), and train students in bioengineering. Future work will extend monitoring and adapt the system for cardiac, renal, and pancreatic preparations, with the longer-term goal of contributing to preclinical perfusion research in settings where commercial NMP systems such as the TransMedics OCS remain financially inaccessible.

DEVELOPMENT OF A SPECIALIZED CLINICAL DECISION SUPPORT SYSTEM FOR HEMOPHILIA-SPECIFIC DRUG INTERACTIONS

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Keywords: Hemophilia, Drug-Drug Interactions (DDI), Clinical Decision Support Systems, Patient Safety, Rare Diseases

Hemophilia is a complex congenital bleeding disorder that requires precise, lifelong therapeutic management. Recent medical advancements have significantly extended the life expectancy of patients, leading to an aging population that increasingly faces age-related comorbidities and the challenges of polypharmacy.

Existing digital tools for checking drug-drug interactions (DDI) provide generic pharmacological data but fail to account for the unique physiological risks and specific contraindications inherent to hemophilia. This study aims to address this safety gap by developing a specialized digital support tool that integrates global pharmacological databases with a custom-built rule engine tailored to the specific needs of patients with bleeding disorders.

The developed tool successfully identifies high-risk interactions specific to hemophilia, which are frequently overlooked by general-purpose platforms, by overlaying a specialized hematological logic engine onto standardized drug APIs.

This application enhances personalized treatment, patient autonomy and provides decision support for non-specialist clinicians. Furthermore, the modular architecture of this tool establishes a scalable framework for improving medication and pharmaceutical safety across various other rare disease domains where specialized pharmacological guidance is currently lacking.

Diagnostic potential of similarity networks in the analysis of T-cell receptor (TCR) repertoires

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Keywords: similarity networks, computational immunology, TCR, heuristic

During their development, each T lymphocyte independently generates a unique receptor sequence through recombination of V, D, and J gene segments. Because this process occurs across a large population of T lymphocytes, it creates a highly diverse set of receptors that together form the T-cell receptor (TCR) repertoire, which changes dynamically depending on the patient's immune response state.

Because TCR repertoires change in response to infection and other immune-related conditions, their analysis has potential diagnostic value. In this work, repertoire features were represented as similarity networks constructed based on distances between receptors, with the aim of identifying an algorithm capable of preserving repertoire properties while enabling distinction between healthy and diseased individuals.

A heuristic approach was developed to identify a combination of network construction algorithms and parameters that generated clearly distinguishable similarity networks for healthy individuals and individuals with COVID-19, achieving an average inter-network distance of 0.7.

These results demonstrate that similarity networks can preserve diagnostically relevant repertoire features and support disease classification. The proposed vector-based network representation also shows potential for method standardization. Future work will extend the approach to other immune-related diseases and develop more advanced methods for network comparison.

EFFECT OF IONIZING RADIATION ON THE HALF-LIFE OF APOPTOSIS-INVOLVED SELECTED PROTEINS IN HCT116 CELLS

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Keywords: data analysis, image analysis, proteins, half-life, cell culture, signaling pathways

Ionizing radiation induces DNA damage and activates the DNA damage response (DDR), leading to alterations in the levels and stability of proteins involved in cell cycle control, DNA repair, and apoptosis.

The tumor suppressor p53 and its downstream effectors, p21 and PTEN, are key regulators of the genotoxic stress response; however, the effects of ionizing radiation on their stability remain incompletely understood. This study aimed to determine the half-lives of these proteins in HCT 116 human colorectal cancer cells under control conditions and after irradiation. Protein stability was assessed using a cycloheximide chase assay combined with Western blot analysis and quantitative signal intensity analysis.

Ionizing radiation differentially modulates protein stability, leading to a prolonged half-life of p21 while maintaining a short half-life of p53 and high stability of PTEN.

These findings demonstrate selective regulation of protein stability in response to genotoxic stress. Improved understanding of these mechanisms may support the development of targeted therapeutic strategies and enhance the effectiveness of radiation-based cancer treatments.

Ethical issues of genomic analysis

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Keywords: genomic analysis, privacy, discrimination, informed consent, bioethics

Genomic analysis plays a critical role in modern biology and medicine, giving insights into disease mechanisms, inheritance, and individual risk profiles. As sequencing technologies become faster and more affordable, their application is quickly expanding beyond research into clinical and commercial settings.

This work examines the ethical implications of genomic analysis through a critical review of documented cases and theoretical frameworks, with particular attention to privacy risks, informed consent, and the potential for genetic discrimination. We analyze how misinterpretation or oversimplification of genetic findings, such as associations between certain variants and aggressive or antisocial behavior, can lead to stigmatization. Additionally, we evaluate existing regulatory approaches and highlight limitations in protecting individuals from misuse of genomic data by employers, insurers, or public institutions.

Our analysis shows that ambiguous interpretation of genotype-phenotype relationships, combined with insufficient legal regulations, creates a risk of discrimination and social harm.

These findings highlight the necessity of integrating ethical standards, clearer communication of genetic risk, and stronger legal protections into genomic research and its applications. Strengthening these frameworks is essential to prevent misuse, ensure equitable treatment, and support responsible advancement in genomics.

EVALUATING EXTRUSION ENERGY CONSUMPTION IN HIGHLY-CONCENTRATED PHOSPHATIDYLCHOLINE LIPOSOMES FORMULATION
PYTHON-BASED SIGNAL PROCESSING APPLICATION

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Keywords: Liposome Extrusion, Energy Consumption, Digital Signal Processing, Python GUI

Liposomes are lipid nanovesicles widely utilized as advanced drug delivery systems to improve drug bioavailability. A common method for vesicle size standardization is extrusion, which involves forcing lipid suspensions through calibrated nanopores. However, high-concentration phosphatidylcholine formulations create significant mechanical resistance, making the sizing process energy-intensive and technically challenging.

Currently, most extrusion research focuses solely on the pressure within the nanopores during the extrusion process as an indicator of its efficiency. This approach ignores the actual mechanical work performed within the lipid system itself, creating a significant research gap in understanding the energetics of membrane deformation induced by extrusion. The goal of this study was to develop a method to determine energy consumption as a function of variable parameters of liposomal formulations, a feat that cannot be achieved solely by standard pressure measurements.

The research resulted in an intuitive Python-based application that determines the net work performed on the lipid membrane by performing trapezoidal numerical integration of the force-time signal difference between the sample and its mechanical background.

By quantifying the actual work done on lipids, rather than the pressure used in the extrusion process, this tool provides a scalable framework for optimizing the production and stability of high-concentration formulations in advanced drug delivery systems.

Evaluation of Portable EEG Metrics as Biomarkers of Rapid Neuroplasticity Induced by Visuomotor Training

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Keywords: EEG, Muse, Neuroplasticity, Visuomotor Training

Neuroplasticity represents the brain's fundamental capacity to reorganise its structure and function in response to experience and learning. While functional MRI is traditionally used to map these changes, portable electroencephalography (EEG) offers a high-temporal-resolution alternative to monitor neural dynamics during cognitive and motor tasks.

Short-term visuomotor training triggers rapid neural adaptations, yet identifying sensitive electrophysiological markers of this process remains a challenge. This study used the Muse EEG system to investigate how quantitative metrics track within-session neuroplasticity across training sessions. Data was collected during a Brainhack event.

In this pilot study involving 9 participants (n=4 control, n=5 experimental), DAR, DTABR, and pdBSI showed negligible group effects and did not reach statistical significance, while the clearest neural signal was found in acute within-session changes. Specifically, Hjorth complexity and mobility, alongside FOOOF spectral slope, emerged as the most robust biomarkers of neural change, reaching statistical significance ($p<.05$, $\eta 2$ up to 0.43).

These findings suggest that temporal-domain and spectral parametrisation metrics may better capture short-term neural fluctuations than conventional band-power ratios. However, due to the small sample size and exploratory design, results should be interpreted cautiously and require validation in larger cohorts.

THE FIRST KONTS IN RNA: BREAKING A STRUCTURAL PARADIGM

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Keywords: RNA topology, RydC sRNA, trefoil knot, molecular dynamics, pseudoknot

The spatial configuration of biopolymers is a fundamental determinant of their biological function and stability. While knots are well-documented in DNA and protein structures, identifying genuine knots in natural RNA molecules has remained an elusive challenge in structural biology.

For decades, it was hypothesized that natural RNAs do not form true topological knots, with previous candidate structures often dismissed as modeling artifacts. This study re-examines experimentally determined RNA 3D structures to identify potential entanglements that may have been overlooked during traditional structural analysis.

We report the discovery of a genuine left-handed trefoil knot (3_1) in the crystal structure of the bacterial small RNA RydC, proving that non-trivial topology can indeed be a feature of natural RNA molecules.

Computational analyses and molecular dynamics suggest that this knotting is a conserved feature of the RydC family and follows a folding pathway similar to that of knotted proteins. These findings challenge existing paradigms in RNA topology and necessitate the inclusion of topological constraints in the development of next-generation RNA 3D structure prediction tools.

From Clinical Markers to Deep Learning: Decoding Trends in Modern Cardiology Using Large-Scale Text Mining and LLM Models

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Keywords: cardiology trends, text mining, large language models, biomarkers

The rapid expansion of cardiovascular medicine has resulted in an unprecedented volume of scientific literature, making it increasingly difficult for researchers to monitor shifting paradigms. Understanding the historical evolution of diagnostic tools and analytical methods is essential for navigating this vast scientific landscape. By identifying long-term patterns, the medical community can better anticipate future directions in clinical research.

Traditional literature reviews are often limited by manual effort and subjective bias, creating a clear need for the automated synthesis of large-scale research trends. This study addresses this gap by utilizing the PubMed API to extract and analyze thousands of abstracts published over the last two decades. The primary objective is to quantify the transition from classic clinical indicators to advanced biomarkers and AI-driven predictive modeling.

By leveraging locally-hosted open-source Large Language Models for automated Named Entity Recognition, the study successfully mapped a definitive temporal shift in cardiology from traditional linear statistics toward complex biomarkers and deep learning algorithms.

This fully automated pipeline demonstrates that the synergy of open-source LLMs and text mining provides a powerful, ethically streamlined method for mapping medical knowledge. Such tools enable rapid synthesis of scientific evidence without requiring access to sensitive patient data. Ultimately, this approach establishes a scalable framework for tracking emerging research frontiers across various medical disciplines.

FROM GUT TO BRAIN - CAN BACTERIA DRIVE AMYLOID PATHOLOGY?

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Keywords: neurodegeneration, gut-brain axis, aggregation, protein interactions

Amyloids are insoluble, fibrillar protein aggregates characterized by a highly ordered β-sheet structure, formed as a result of protein misfolding. Their accumulation is a hallmark of numerous neurodegenerative disorders (NDDs), including Alzheimer's disease (tau and Aβ), and Parkinson's disease (α-synuclein).

The human body is colonized by a complex microbiome comprising both beneficial and pathogenic bacteria. Notably, many bacteria produce functional amyloids, such as curli in *Escherichia coli* and FapC in *Pseudomonas strains*, which play structural roles but may also interact with host proteins. Emerging evidence indicates a connection between microbiome and NDDs, potentially mediated by the gut-brain axis. For example, *Helicobacter pylori* infection has been associated with both Alzheimer's and Parkinson's diseases.

In my studies, I investigate interactions between selected bacterial proteins and amyloids associated with NDDs, using a range of bioinformatic and experimental techniques, including AlphaFold 3, aggregation predictors, electron microscopy (EM), thioflavin T (ThT) fluorescence assay, circular dichroism (CD) and attenuated total reflectance Fourier-transform infrared (ATR-FTIR) spectroscopies. Elucidating these interactions may provide insight into the mechanisms underlying protein aggregation and interaction, ultimately contributing to the identification of novel therapeutic targets and strategies for the prevention and treatment of NDDs.

FROM HEALTH TO ADENOMA TO COLORECTAL CANCER: EXPLORING GUT MICROBIOME SIGNATURES

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Keywords: gut microbiome, adenoma, colorectal cancer, bioinformatics

Gut microbiome plays a key role in maintaining homeostasis and regulating proper intestinal function. The shifts in its composition may indicate a severe disease with a high mortality rate, such as colorectal cancer (CRC). The early diagnosis of the precancerous stage - adenoma, requires a colonoscopy, which is an invasive procedure. Understanding the changes that happen inside the gut microbiome will aid prevention and early detection by using more accessible non-invasive methods.

Despite significant progress in colorectal cancer research, robust microbiome markers based on quantitative and qualitative analyses have not yet been firmly established. We performed a cross-study analysis on 2165 microbiome samples collected within 24 independent studies, in order to identify microbiome-derived markers that could play a fundamental role in colorectal cancer progression.

Preliminary results did not reveal significant differences in the microbiome composition between the study groups. However, we observed that the microbiome functions are more stable than taxonomic composition, suggesting that functional profiles should be analysed further. Moreover, the effect of geographic location where one lives may have a greater influence on colorectal cancer development.

Identifying gradual microbial changes may improve screening strategies and enable early intervention, helping reduce the number of colorectal cancer cases and deaths.

FROM MOLECULAR BRICKS AND A WHOLE-CELL MODEL TO A DIGITAL TWIN

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Keywords: virtual cell, multi-omics, synthetic life

A whole-cell model is a computational model that simulates an entire living cell, mimicking interactions between cellular components including nucleic acids, genes, proteins, and regulatory or metabolic networks.

Traditional approach based on biochemical analyses provided limited information in spatiotemporal resolution not allowing understanding of dynamic biological activities on different scales. Advances in artificial intelligence (AI) led to the AI virtual cell (AIVC). By combining different types of biological data (“multi-omics”) with methods from many scientific fields, AIVC creates a digital copy of a cell that can simulate its functions and behavior.

Recent studies have introduced a whole-cell computational model that simulates an entire cell cycle in four dimensions (space and time) and integrates gene expression, metabolism, growth, chromosome replication, and cell division, reproducing many experimentally observed features, such as protein distributions, ribosome numbers, and DNA replication dynamics. They revealed that even genetically identical cells can behave differently because of stochastic biological processes.

Such “virtual cells” may become a powerful platform for testing biological hypotheses, predicting cellular behavior, and designing synthetic or engineered life systems in silico. These advances pave the way for developing cellular digital twins that could support personalized medicine predicting how cells respond to diseases, drugs, or therapies.

THE GIFT FROM THE OCEAN – PHARMACOLOGICALLY ACTIVE COMPOUNDS FROM MARINE HYDROBIONTS

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Keywords: carrageenans, chitosan, marine polysaccharides, immunomodulation

Marine polysaccharides, particularly sulfated carrageenans from red algae and chitosan derived from chitin, have evolved from industrial materials into biologically active compounds with significant immunological relevance. Beyond their traditional uses, they engage in a complex interplay with the immune system, balancing activation and regulation.

This study explores how structural features dictate biological function. Subtle variations, such as sulfation patterns in carrageenans and the molecular weight and degree of acetylation in chitosan, serve as critical determinants of activity. Using approaches ranging from in vitro systems to in vivo models, their immunomodulatory, anti-inflammatory, antiviral, anticoagulant, and antitumor properties were evaluated.

Depolymerisation acts not merely as degradation but as functional transformation. Carrageenans modulate inflammatory responses while preserving anti-inflammatory cytokine production, supporting immune balance. In chitosan, depolymerisation enhances biological activity, strengthening antiviral responses and cytokine induction.

These findings highlight that biological activity depends not only on composition but also on molecular architecture. Marine polysaccharides thus represent tunable biomolecular systems with strong potential for developing therapies targeting inflammation, infection, and cancer.

Hacking Parkinson's Disease: Gene Editing and the Next Therapeutic Revolution

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Keywords: Parkinson's disease, gene therapy, CRISPR-Cas9, neuroprotection

In light of the limited effectiveness of traditional treatments for Parkinson's disease (PD), there is a growing demand for innovative therapies capable of modifying the course of the disease. This review focuses on modern approaches, including gene-editing technologies (such as CRISPR-Cas9), vector-based delivery systems, and immunotherapeutic strategies aimed at slowing neurodegenerative processes and supporting the function of dopaminergic neurons.

This paper is a narrative review that presents the main directions of current research in this field, while also identifying key challenges associated with the development and implementation of these therapies. It discusses general research strategies and their underlying mechanisms, as well as limitations such as the difficulty of efficiently delivering genetic material to the central nervous system, particularly across the blood–brain barrier, and the potential for immune responses. The aim of this work is to provide a concise synthesis of the current state of knowledge and to highlight the major issues that will shape the future development of innovative therapies for Parkinson's disease.

HIGH DICE, BROKEN VESSELS: EVALUATING TOPOLOGY ERRORS IN DEEP LEARNING VESSEL SEGMENTATION

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Keywords: vascular segmentation, topology-aware metrics, dice similarity coefficient

Deep learning methods have achieved state-of-the-art performance in vascular segmentation from CT images, commonly evaluated using overlap-based metrics such as the Dice similarity coefficient1. However, vascular structures form complex tree-like topologies, where small segmentation errors can disrupt vessel continuity while still yielding high Dice scores. Such errors limit the clinical usability of automatic vessel segmentation for applications including surgical planning, hemodynamic modeling, and quantitative vascular analysis. This study investigates limitations of Dice-based evaluation for vascular segmentation and quantifies topology-related segmentation failures across multiple public datasets.

Segmentation models were trained using the nnU-Net framework1 on four publicly available vascular CT datasets: SEGA, AortaSeg24, PARSE2022, and TopCoW2024. Predicted segmentations were compared with ground-truth annotations using both conventional and topology-aware metrics. These metrics quantify structural inconsistencies such as vessel fragmentation, missing branches, and disconnected components.

Across all datasets, models frequently achieved high Dice scores (>0.9 in many cases) despite significant topological errors in the predicted vascular structures. Common malfunction included fragmented vessels, disconnected branches, and artificial components. In many cases, predicted segmentations contained substantially more disconnected components than ground truth, indicating broken vessel continuity. Topology-aware metrics revealed structural errors not captured by Dice similarity.

These findings highlight a critical limitation of Dice-based evaluation for vascular segmentation. Although deep learning models may achieve high overlap scores, their predictions often contain topological inconsistencies that undermine clinical usability. Topology-aware metrics provide a more informative assessment of vascular segmentation quality and should complement traditional overlap measures.

IMPROVING WHOLE EXOME SEQUENCING INTERPRETATION IN INFERTILITY THROUGH EVIDENCE BASED LITERATURE INTEGRATION PIPELINE

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Keywords: infertility, Whole Exome Sequencing, variant interpretation, reproductive genetics

Infertility is a multifactorial disorder affecting millions worldwide, with genetic factors contributing substantially to both female and male reproductive dysfunction. Although Whole Exome Sequencing (WES) enables large-scale detection of genomic variation, translating raw sequencing data into clinically meaningful findings remains challenging.

A key limitation of current diagnostic workflows is the gap between rapidly expanding scientific literature and routinely used variant interpretation resources. Many potentially relevant single nucleotide polymorphisms remain classified as variants of uncertain significance (VUS) or are overlooked entirely. To address this, we developed an internal literature integration pipeline that systematically screens, curates and prioritizes publications describing infertility associated polymorphic variants. The tool functions as a publication gating system that selects high value evidence and enables targeted identification of candidate SNPs potentially linked to infertility.

The strategy is expected to significantly improve detection of clinically relevant variants by revealing evidence supported SNPs missed by conventional database approaches.

This strategy may reduce interpretative uncertainty, accelerate genomic diagnostics, and support more personalized reproductive counseling and treatment decisions. More broadly, it demonstrates how structured literature mining can strengthen variant classification and advance precision medicine in reproductive genetics.

INFLUENCE OF DISTAL SUPPORT ON THE BIOMECHANICAL BEHAVIOR OF MAXILLARY FULL-ARCH PROSTHESES: A FINITE ELEMENT STUDY

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Keywords: full dental arch, tubero-pterygoid implant, maxillary distal support, Finite Element Method (FEM)

Edentulism is a significant social and health concern. The increasing use of implant-supported prosthetic rehabilitation, combined with difficulties in achieving distal support in the maxilla, makes the design of full-arch restorations a distinct clinical challenge.

Achieving proper distal support in the maxilla remains difficult and the biomechanical performance of different implant configurations is not yet fully established. In this study, two geometric models were developed: M4, representing a four-implant-supported fixed prosthesis, and M6, a six-implant-supported design including additional tubero-pterygoid implants in the distal region. The aim of the study was to evaluate which configuration provides greater stability and safety for the patient.

The results indicated superior biomechanical stability of the prosthesis-implant-bone system, as well as reduced stress and strain on the prosthetic components and bone in the M6 model. It was also observed that a lack of distal support may cause anterior implants to be pulled out of the bone and posterior implants to be pushed into the bone, particularly during central occlusion in the M4 model.

Therefore, tubero-pterygoid implants are an effective method for increasing the stability of full-arch prostheses. Future studies should include an extension of numerical analyses to dynamic and fatigue simulations, as well as experimental investigations using a drop-weight impact tester and an MTS machine.

INVESTIGATING POTENTIAL THERAPEUTICS FOR MELANOMA VIA THE MTOR SIGNALING PATHWAY USING PETRI NET MODELING

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Keywords: Petri Nets, mTORC signaling pathway, therapeutic target identification, uveal melanoma metastasis

The mTORC signaling pathway plays a central role in regulating cell growth, metabolism, and survival. Its dysregulation has been widely implicated in cancer progression, including metastasis. Petri nets are a mathematical and graphical modeling formalism used to describe and analyze distributed, concurrent, and dynamic systems, and have been successfully applied to the study of biological pathways.

Despite extensive research on mTORC signaling, the mechanisms underlying metastatic progression, particularly in uveal melanoma, remain incompletely understood. In this study, we used a Petri net–based model of the mTORC signaling pathway to perform knockout and MCT analyses, aiming to identify key regulatory elements and potential therapeutic targets.

The Petri net model exhibited biologically consistent behavior, and knockout and MCT analyses identified key components whose disruption significantly alters network dynamics, indicating their potential role in metastatic progression and therapeutic targeting.

This study demonstrates the usefulness of Petri net–based approaches in uncovering critical vulnerabilities in complex biological networks. The results contribute to a better systems-level understanding of mTORC signaling in uveal melanoma and may support future research in the development of targeted therapies.

INVESTIGATING THE THERMOSTABILITY OF MINIPROTEINS THROUGH CIRCULAR DICHROISM SPECTROSCOPY

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Keywords: miniprotein, secondary structure, characterization, polarization, conformational stability

Miniproteins – the polypeptides that remain characteristics of functional proteins despite their molecular mass smaller than 10 kDa, have been gaining importance in protein folding modelling and engineered protein-based therapeutics fields. Therefore, the aim of this study was to analyze the secondary thermal structure stability of *ALL*, *MV* and *MvaT* miniproteins promising in designing scaffolds for developing enzyme-like catalysts applications [1] using circular dichroism (CD) spectroscopy.

The stability was investigated over the temperature range of 4 °C–96 °C after dissolution of the miniproteins in Tris-HCl buffer at pH 7.2. The measurements of the *ALL* and *MV* at 25°C indicated that their secondary structure consisted predominantly of regular α-helices.
In the case of *MvaT*, a significant contribution of antiparallel β-sheets with right-handed twist was also observed. Heating all samples from 4 °C to 96 °C revealed an increase in the share of the antiparallel β-sheet with right-handed twist in the solution compared to the contribution of the regular parts of helices. However, after the process of recooling to 25 °C, the larger share for the regular helix parts side was again observable.

The partial recovery of the initial secondary structure after recooling suggests that the investigated miniproteins fold cooperatively and preserve a considerable degree of conformational stability despite exposure to high temperatures.

[1] Rudzińska-Szostak, E., & Berlicki, Ł. (2026). Towards filling the gap between organocatalysis and biocatalysis – catalysis by folded peptides and miniproteins. Tetrahedron Chem, 100161, https://doi.org/10.1016/j.tchem.2026.100161.

A NOVEL POLISH MEDICAL CORPUS FOR DOMAIN-ADAPTIVE LLMS TRAINING

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Keywords: Polish medical corpus; Large Language Models; domain-adaptive pretraining; Natural Language Processing; Polish-DistilRoBERTa

Large general-domain corpora serve as a powerful resource for LLMs training. When adapting to selected fields, LLMs can be further trained on domain-specific corpora that contain specialized vocabulary. This study addresses the lack of Polish medical corpora by developing a domain-specific dataset focused on infertility, genetics, and gynecology, designed for domain-adaptive pretraining of language models.

To achieve this goal, medical text data was selected and pre-processed. The corpus was constructed using three approaches, two of which were based on publicly available tools, and the third involved an original method. The primary corpus file underwent post-processing for standardization. The final corpus with over 4 million words was used for continuous domain-adaptive pretraining of the Polish-DistilRoBERTa model using the Masked Language Modeling (MLM) method. Subsequently, the MLM loss function was used to evaluate the usefulness of the final corpus.

A decrease in MLM loss and similar trends in both validation and training curves confirm the effectiveness and suitability of the constructed corpus for domain adaptation. The developed language model will be used in clinical data classification, enabling more efficient NLP-based analysis.

Acknowledgements:
The project was conducted in cooperation with the Genetic Laboratory of the Gyncentrum Sp. z o.o. in Sosnowiec. This work was supported by the Ministry of Science and Higher Education 'Implementation Doctorate' grant number DWD/7/0396/2023.

LABEL-FREE QUANTITATIVE IMAGING REVEALS RED BLOOD CELL SUBPOPULATIONS ASSOCIATED WITH AGING

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Keywords: red blood cells, digital holotomography, segmentation

Erythrocytes constitute approximately 40–45% of total blood volume, serving as primary carriers of oxygen and carbon dioxide and as indicators of systemic homeostasis [1]. The morphology of red blood cells (RBCs) may reflect various pathological conditions and disease states, as well as functional alterations associated with aging [1,2]. This underscores the need for quantitative RBC characterization, enabling the identification of distinct morphologies and the extraction of relevant parameters.

In this study, digital holotomography (DHT) was employed for the quantitative characterization and segmentation of RBC morphologies associated with aging. Tomograms of RBCs, representing the spatial distribution of refractive index (RI) within the sample, were analyzed using a custom Python-based workfow. The developed approach enabled RBC segmentation, identification of morphology-based subpopulations, and extraction of quantitative descriptors from reconstructed tomograms.

The proposed software provides flexible adjustment of key parameters in tomogram analysis. Moreover, the extracted quantitative descriptors of RBCs may serve as a basis for the development of machine learning (ML)-based approaches for segmentation and classification in future applications.

References:

1. *Paul R et al. RSC Adv. 2020;10(64):38923–38936. doi:10.1039/d0ra05421f*
2. *Massaccesi L et al. Mech Ageing Dev. 2020;191:111333. doi:10.1016/j.mad.2020.111333*

LINKING AMYLOIDOGENIC POTENTIAL, FUNCTION, AND STRUCTURE IN A BIOINFORMATIC STUDY OF PRION PEPTIDES

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Keywords: amyloidogenic peptides, prion peptides, protein aggregation, bioinformatic analysis

Peptides with amyloid properties are the subject of scientific research due to their distinctive biochemical characteristics, which lead to the formation of pathogenic aggregates as well as stable functional structures. They are often hydrophobic and rich in β-sheet structures, forming cross-β architectures.

Although predictors of amyloidogenic potential currently exist, there is still a lack of tools that integrate detailed features of spatial structure with the actual molecular functions of peptides. Bioinformatic analysis of these molecules may help identify integrated functional, sequential, and structural patterns that could prove useful in detecting amino acid motifs with similar properties.

Examined peptides were suspected of having aggregation properties, because they originate from prion proteins; however, despite some structural characteristics indicating amyloidogenicity, predictions from several bioinformatic tools showed, that those peptides demonstrate little to none proneness to aggregation.

These results should be interpreted with caution, as they are based on bioinformatic predictions, which cannot fully capture the complexity of peptide behavior in biological systems. Therefore, such predictions should not be treated as definitive and the conclusions regarding amyloidogenicity, require experimental validation. Nevertheless, these tools are valuable for preliminary examination of the peptides, as they can support and complement experimental findings. In particular, the prediction of Aggregation Prone Regions (APRs) and secondary structure provides useful insights, that would otherwise require more complex techniques, such as, for instance, X-ray crystallography or cryogenic electron microscopy.

LONGITUDINAL ANALYSIS OF SINONASAL MICROBIOME IN CHRONIC RHINOSINUSITIS

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Keywords: microbiome, chronic rhinosinusitis, long-read sequencing, personalized medicine

Most studies on the sinonasal microbiome were conducted at a single time point and limited to genus-level resolution, leaving the temporal dynamics of the microbial community in this niche poorly understood. Chronic rhinosinusitis (CRS) is among the most prevalent chronic inflammatory diseases of the upper airways, yet the role of the microbiome in disease progression and acute exacerbations remains unclear.

We collected longitudinal sinonasal samples from CRS patients at a minimum of four time points, alongside samples from healthy controls. Full-length 16S rRNA gene sequencing was performed using Oxford Nanopore Technologies, enabling species-level taxonomic resolution. Sequencing-based profiles were compared with results from routine hospital microbiological cultures.

The sinonasal microbiome exhibited high inter-individual variability in both CRS patients and healthy controls, with no consistent taxonomic signatures distinguishing the two groups. Within the heterogeneous CRS cohort, shifts in microbiome composition and temporal dynamics coincided with episodes of symptom worsening in a subset of individuals. Building on these observations, we developed an approach to identify microbial blooms associated with bacterial exacerbations.

Our work demonstrates how advanced sequencing technologies can enhance clinical diagnostics and bring us a step closer to precision medicine. This research was funded by the National Science Centre, Poland, grant number 2023/51/D/NZ5/01206

METAGENOMICS-DRIVEN ALGORITHM FOR PRECISION DIAGNOSIS OF SMALL INTESTINAL DYSBIOSES

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Keywords: SIBO, metagenomics, molecular diagnostics, microbiome biomarkers

Small intestinal dysbioses, including small intestinal bacterial overgrowth (SIBO), intestinal methanogen overgrowth (IMO), hydrogen sulphide overgrowth (ISO) and small intestinal fungal overgrowth (SIFO) are increasingly recognised as important contributors to chronic gastrointestinal disorders and systemic symptoms mediated through the gut–brain axis. Advances in microbiome research have highlighted the need for precise and mechanism-based diagnostic approaches capable of characterising the complex microbial ecosystem of the small intestine.

Current diagnostic methods rely predominantly on indirect breath testing or culture-based techniques, which are limited by insufficient sensitivity, specificity and inability to comprehensively characterise microbial composition and function. This ongoing translational research project aims to develop a multi-layer diagnostic algorithm for small intestinal dysbioses by integrating shotgun metagenomics of small intestinal aspirates, 16S rRNA profiling and genome-resolved analyses. The study focuses on identifying taxonomic and functional biomarkers linked to key microbial metabolic pathways, including methanogenesis and hydrogen sulphide production, and translating these findings into quantitative real-time PCR assays suitable for routine clinical diagnostics.

The proposed framework enables precise molecular stratification of dysbiosis subtypes and supports personalised therapeutic decision-making. By replacing indirect gas-based diagnostics with microbiome-informed molecular tools, this approach may improve treatment outcomes, reduce empirical therapies and advance precision medicine targeting the small intestinal microbiome.

MITIGATING ANNOTATION BOTTLENECKS IN KI-67 QUANTIFICATION VIA TEACHER-STUDENT PSEUDO-LABELING

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Keywords: Ki-67 Index, Pseudo-Labeling, Tissue Segmentation, Digital Pathology

Precise diagnosis and treatment planning are essential for successful cancer care. In breast cancer pathology, the Ki-67 index is a key marker used to measure how fast tumor cells grow. However, estimating this index manually is slow and often varies between different pathologists. Although deep learning based pipelines can automate this task, the training of these models requires many manually labeled images, which are very costly and time-consuming in acquisition. To solve this problem, we developed a semi-supervised method that combines a small amount of expert data with a large pool of unlabeled images. The main objective was to create a system that segments tumor tissue and individual cell nuclei without relying on heavy human labor. Our final model accurately segments tumor tissue with an F1-score of 0.85 and predicts the overall Ki-67 index with a mean absolute error of 4.1% and a high intraclass correlation coefficient of 0.97 compared to expert pathologists.

These findings demonstrate that deep learning models can be successfully trained while minimizing manual annotation constraints. This approach significantly simplifies the adaptation of digital pathology systems to diverse laboratory staining and imaging conditions, ultimately facilitating more reliable automated cancer diagnostics in clinical workflows.

MOLECULAR DYNAMICS STUDY OF 2,6-DIAMINOPURINE IN NONENZYMATIC RNA REPLICATION

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Keywords: non-enzymatic self-replication, molecular dynamics, 2,6-diaminopurine, prebiotic chemistry

How life first emerged on Earth remains one of the biggest open questions in science. One widely accepted hypothesis suggests that RNA, due to its ability to store genetic information and catalyze chemical reactions, played a key role in early life. Studying how RNA replicated before enzymes existed may help uncover the very first stages of the emergence of living matter [1]. Nonenzymatic RNA replication uses chemically activated nucleotides, with imidazolium-bridged dinucleotides as key reactive intermediates. Primer extension efficiency depends on the O3′-P distance, attack angle, and Watson-Crick base pairing [2]. Replacing adenine with 2,6-diaminopurine (D) improves base pairing with uracil, resulting in three hydrogen bonds, thereby enhancing template binding and increasing copying efficiency [3]. However, the structural dynamics of D-containing activated dinucleotides remain poorly understood.

Molecular dynamics simulations reveal that the imidazolium-activated D dinucleotide maintains stable Watson-Crick pairing with the uracil template. Throughout the simulation, the system commonly adopts short O3′-P distances and suitable attack angles, indicating favorable conditions for nonenzymatic RNA self-replication. These results indicate that stable base-paired geometry is associated with reactive conformations that promote primer extension, which may explain the increased yield and fidelity of RNA self-replication with D-containing substrates.

References:

[1] M. P. Robertson, G. F. Joyce, The Origins of the RNA World, *Cold Spring Harb. Perspect. Biol.*, 2012, 4, a003608.
[2] T. Walton, W. Zhang, L. Li, C. P. Tam, J. W. Szostak, The Mechanism of Nonenzymatic Template Copying with Imidazole-Activated Nucleotides, Angew. Chem. Int. Ed. 2019, 58, 10812–10819.
[3] X. Jia, Z. Fang, S. C. Kim, D. Ding, L. Zhou, J. W. Szostak, Diaminopurine in Nonenzymatic RNA Template Copying, J. Am. Chem. Soc. 2024, 146, 15897–15907.

A Novel Polish Medical Corpus for Domain-Adaptive LLMs Training

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Keywords: Polish medical corpus; Large Language Models; domain-adaptive pretraining; Natural Language Processing; Polish-DistilRoBERTa

Large general-domain corpora serve as a powerful resource for LLMs training. When adapting to selected fields, LLMs can be further trained on domain-specific corpora that contain specialized vocabulary. This study addresses the lack of Polish medical corpora by developing a domain-specific dataset focused on infertility, genetics, and gynecology, designed for domain-adaptive pretraining of language models.
To achieve this goal, medical text data was selected and pre-processed. The corpus was constructed using three approaches, two of which were based on publicly available tools, and the third involved an original method. The primary corpus file underwent post-processing for standardization. The final corpus with over 4 million words was used for continuous domain-adaptive pretraining of the Polish-DistilRoBERTa model using the Masked Language Modeling (MLM) method. Subsequently, the MLM loss function was used to evaluate the usefulness of the final corpus.
A decrease in MLM loss and similar trends in both validation and training curves confirm the effectiveness and suitability of the constructed corpus for domain adaptation. The developed language model will be used in clinical data classification, enabling more efficient NLP-based analysis.

Acknowledgements: The project was conducted in cooperation with the Genetic Laboratory of the Gyncentrum Sp. z o.o. in Sosnowiec. This work was supported by the Ministry of Science and Higher Education ‘Implementation Doctorate’ grant number DWD/7/0396/2023.

PETRI NET-BASED MODELING AND SIMULATION OF P13K-AKT THERAPEUTIC TARGETING

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Keywords: Petri net modeling, P13K-Akt signaling pathway, Novel simulation framework, In silico therapeutic modeling

A Petri net is a mathematical model that can be represented as a weighted directed bipartite graph. It is particularly well suited for modeling complex and dynamic systems, including biological processes. Due to its intuitive graphical representation and formal rigor, this approach has gained increasing popularity in systems biology.

The growing interest in applying Petri nets to biological systems stems from their ability to naturally capture the structure and behavior of biochemical processes. Petri nets enable flexible modeling of complex systems, combining formal precision with a clear graphical structure. However, there remains a need for improved methods to simulate and statistically evaluate complex biological pathways, particularly under varying conditions such as therapeutic interventions or mutations. This study aims to develop a novel method for simulation and statistical testing of such systems, enabling the introduction of perturbations and systematic observation of resulting behaviors.

A complete Petri net model of the P13K-Akt signaling pathway was developed and validated, demonstrating that simulations of two therapeutic interventions produced results consistent with existing literature while also revealing novel insights beyond experimental observations.

These findings contribute to advancing computational modeling approaches in systems biology by providing a robust and interpretable framework for analyzing complex signaling pathways. The proposed method enables more comprehensive in silico experimentation, potentially reducing the need for costly and time-consuming laboratory studies. Furthermore, it opens new opportunities for predicting the effects of therapies and mutations, supporting the development of more effective and personalized treatment strategies.

POMOKA: An Integrated Clinical Decision Support Platform for Cardiac Surgery

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Keywords: cardiac surgery, clinical decision support, survival analysis, machine learning

Cardiac surgery requires precise, data-driven tools to accurately assess patient outcomes and optimize surgical strategies. Clinical decision support systems are increasingly utilized to evaluate complex health metrics and predict patient trajectories. By leveraging advanced statistical and computational methods, these platforms can significantly enhance clinical decision-making.

Direct survival comparisons between specific clinical cohorts and reference populations are often hindered by incompatible data structures, while accurately estimating perioperative mortality requires robust predictive modeling. To address these methodological gaps, the POMOKA web application was developed as a clinical decision support platform for cardiac surgeons. Its primary objective is to provide dedicated, accessible modules for both advanced survival analysis and precise perioperative risk calculation.

The developed system successfully resolved data structure incompatibilities to enable direct Kaplan-Meier survival comparisons with general population statistics, while concurrently deploying an optimized machine learning model built via rigorous feature engineering and data imputation that accurately estimates patient risk based on operative factors.

By translating complex statistical methodologies into an accessible web-based tool, POMOKA bridges the gap between raw healthcare data and clinical utility. This enables cardiac surgeons to proactively adjust operative procedures based on individualized risk assessments. Ultimately, the platform establishes a practical framework for integrating population-level statistics and predictive machine learning directly into specialized surgical workflows.

PROTO-NOOS: COMPARATIVE ANALYSIS OF ECDHFR–NADPH–LIGAND COMPLEX DYNAMICS FOR SELECTED TRIMETHOPRIM ANALOGUES

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Keywords: Dihydrofolate reductase, Trimethoprim, Molecular dynamics, machine learning

Escherichia coli dihydrofolate reductase (EcDHFR) is a well-established antibacterial target, and trimethoprim serves as the reference compound for inhibitor design. Ligand recognition by EcDHFR cannot, however, be reliably described by docking alone, as it depends on protein dynamics, NADPH occupancy, ligand-residue contacts, and conformational changes within the M20 loop.

In this work, we present a comparative analysis of EcDHFR–ligand complexes for trimethoprim analogues selected as EcDHFR inhibitors by the PROTO-NOOS system. PROTO-NOOS enables the identification of promising compounds but does not encompass in-depth dynamic or energetic analysis; the proposed approach fills this gap. The EcDHFR–TMP–NADPH system is treated as the reference for candidate evaluation. PyMOL is used for preparation and quality control of input structures for molecular dynamics.

Molecular dynamics simulations in GROMACS are used to assess binding mode stability, protein and ligand RMSD, M20 loop RMSF, persistence of intermolecular contacts, hydrogen bonds, and pocket solvent accessibility. For selected systems, PLUMED will be applied for metadynamics, enabling reconstruction of ligand dissociation free-energy profiles and identification of metastable binding modes. This work extends PROTO-NOOS with a chemical, dynamic, and energetic layer, supporting more rigorous selection of antibacterial compounds.

PROTO-NOOS: ORCHESTRATING OPEN-ACCESS BIOINFORMATICS FOR SEAMLESS DRUG DISCOVERY

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Keywords: Computational drug discovery, De novo molecule generation, Machine learning, In silico pipeline

Drug design increasingly relies on in silico methods, yet powerful tools remain scattered across incompatible environments with steep learning curves. We present PROTO-NOOS, a modular pipeline covering the full workflow from hit generation and optimization to in silico semi-validation, with CP2K quantum chemical analysis as the only remaining step before wet-lab verification.

PROTO-NOOS is an 8-stage pipeline designed for benchmarkability and straightforward biological target substitution. We generated a de novo compound dataset targeting EcDHFR and reprocessed data from Stokes et al. (2020) to assess phenotypic concordance, cross-referencing ChEMBL and BindingDB activity data.

The pipeline integrates six freely available tools — GROMACS, Boltz-2, COBRApy, BioTransformer3, REINVENT4, and AiZynthFinder — alongside an efflux prediction model, ODE-based pharmacokinetic models, and Python filtering scripts. Over 20,000 de novo compounds were labeled for machine learning. ODE parameter calibration using experimental data demonstrates the value of target-specific kinetic fitting.

PROTO-NOOS produces results competitive with state-of-the-art open-access alternatives without a commercial license. Preliminary results match Stokes dataset benchmarks, most characterized ligands are correctly ranked, and EcDHFR ODE calibration was achieved successfully. This pipeline is particularly relevant for research groups lacking the infrastructure or expertise to configure and deploy individual computational tools for a specific biological target.

PROTO-NOOS: RATIONAL COMPUTE ALLOCATION IN ANTIBIOTIC DISCOVERY VIA MUTUAL INFORMATION AND UNCERTAINTY QUANTIFICATION

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Keywords: Machine Learning, Mutual Information, Uncertainty Quantification, Drug Discovery

Small-molecule antibiotic discovery suffers from hit rates below 10% and escalating costs when multi-stage pipelines evaluate all candidates uniformly. Rational compute allocation requires knowing how much each stage contributes to the final biological verdict.

We present a systematic ML analysis of the PROTO-NOOS pipeline targeting E. coli dihydrofolate reductase (EcDHFR), spanning generative chemistry, pharmacokinetics, molecular dynamics, and flux-balance analysis. We assessed whether stagewise mutual information (MI) and calibrated uncertainty quantification can replace downstream computations without sacrificing hit quality.

Stagewise MI was estimated using MIST-QR, with KSG as a non-parametric baseline. Chemprop D-MPNN surrogates with Normal-Inverse-Gamma evidential uncertainty heads were trained on partial pipeline observations; early-exit policies were gated on epistemic uncertainty thresholds, with OOD detection via Tanimoto similarity. The benchmark uses 779 EcDHFR inhibitors and 2,335 Stokes et al. (2020) compounds for validation.

MI analysis revealed near-zero information gain from docking and cell-engagement stages toward FBA-based growth inhibition. Conformal prediction achieved nominal pseudo-label coverage but degraded under distribution shift. REINVENT4-generated compounds diverge from experimental distributions, limiting label transfer. Binding affinity is insufficient as a primary criterion; uncertainty-gated early-exit policies offer a principled, budget-aware framework applicable to any CADD pipeline where surrogate reliability under distribution shift must be monitored.

REPROGRAMMING CELLS WITH AI: CONTROLLING GENE REGULATORY NETWORKS

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Keywords: Network Control, Boolean Networks, Deep Reinforcement Learning, Cellular Reprogramming

Cellular reprogramming – the directed conversion of one cell type into another – has emerged as a promising approach for understanding and treating complex diseases. By steering cells toward desired phenotypes, it offers potential applications in regenerative medicine and disease modelling. However, identifying effective reprogramming strategies remains a major challenge.

Experimental discovery of such strategies through wet-lab approaches is often time-consuming and costly, motivating the development of computational methods. In this work, gene regulatory networks are modelled using Boolean Networks, and the search for reprogramming strategies is formulated as a control problem. Due to the computational complexity of identifying optimal control policies, we propose a novel framework based on deep reinforcement learning to efficiently explore network dynamics and identify candidate interventions.

Our results show that the proposed deep reinforcement learning framework significantly improves the computational tractability of identifying effective (optimal or near-optimal) control strategies for cellular reprogramming.

These findings demonstrate the potential of combining network-based modelling with modern machine learning to address challenging control problems in systems biology. The proposed approach contributes to advancing computational tools for cellular reprogramming and may accelerate the discovery of therapeutic strategies. More broadly, it highlights how reinforcement learning can be leveraged to tackle complex decision-making problems in biological systems.

REPROGRAMMING THE HEART: LIPID NANOPARTICLES IN CARDIAC REPAIR

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Keywords: lipid nanoparticles, myocardial infraction, gene therapy, nanomedicine

Ischemic heart disease, frequently culminating in myocardial infarction (MI), remains the leading cause of mortality among cardiovascular disorders worldwide [1]. Despite advances in acute care, post-MI patients continue to face poor long-term prognosis due to the limited regenerative capacity of adult cardiac tissue [2].

Recent evidence indicates that neonatal human hearts possess a transient ability to regenerate cardiac tissue, which is rapidly lost after birth [3]. This finding has inspired the development of therapeutic strategies aimed at reactivating cardiomyocyte proliferation in the adult myocardium. The REGeRNA project, a multidisciplinary European consortium funded under the Horizon program, seeks to develop gene therapy approaches targeting metabolic and regulatory pathways involved in cardiomyocyte cell cycle re-entry.

Within this framework, Lipid Systems sp. z o.o. is responsible for the development of lipid nanoparticle (LNP)-based delivery systems for efficient RNA encapsulation and targeted delivery to infarcted cardiac tissue. The company has demonstrated high mRNA encapsulation efficiency and successful in vitro transfection, and is currently advancing strategies for tissue-specific delivery to the heart.

Overall, REGeRNA represents a promising translational strategy for cardiac regeneration, addressing key limitations of current post-MI therapies through the integration of gene therapy and nanomedicine.

References:

1. *Mensah GA et al., Global Burden of Cardiovascular Diseases and Risks, 1990–2022. J. Am. Coll. Cardiol. 2023, 82, 2350–2473. https://doi.org/10.1016/j.jacc.2023.11.007*
2. *Bayat S et al., Long-Term Survival Rate Following Myocardial Infarction and the Effect of Discharge Medications on the Survival Rate. J. Res. Health Sci. 2022, 22, e00567.*
3. *Haubner BJ et al., Functional Recovery of a Human Neonatal Heart After Severe Myocardial Infarction. Circ. Res. 2016, 118, 216–221. https://doi.org/10.1161/CIRCRESAHA.115.307017*

RESEARCH EXCELLENCE AND THE FUTURE OF BIOINFORMATICS AND COMPUTATIONAL MEDICINE

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Keywords: bioinformatics, computational biology, computational medicine, academia, industry, interdisciplinary research, research excellence

Bioinformatics and computational medicine are coming of age as important interdisciplinary branches of science. From the early days of Margaret Dayhoff's pioneering work in the 1960s, bioinformatics has steadily aided biology, until now, when it is in a position to transform it radically. Computational work is no longer merely supporting experimental biology and medicine; instead, it is increasingly driving discovery and innovation in fields where reliance on experimental work alone would render research inefficient or entirely intractable – for example in drug and protein design, in multi-omics, or in genomics studies. Because bioinformatics is inherently interdisciplinary, it requires particular care and attention to research excellence. Correctly identifying, addressing and testing research hypotheses, communicating with the target audience, diligent resource management and a clear understanding of ethical considerations are becoming increasingly important in carrying out cutting-edge interdisciplinary research. Community support through training and education, access to resources and infrastructure, and the development of shared standards and best practices are equally essential to nurturing the next generation of researchers and to sustaining the field's momentum. In my talk, I will reflect on what research excellence means in this context, and on the role our community must play in shaping the future of the field.

RNALOOPS 2.0: A PLATFORM FOR EFFICIENT SEARCHING OF MULTI-BRANCH RNA LOOP STRUCTURES

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Keywords: RNA structural motifs, multiloops, RNA modelling, database

RNA molecules exhibit complex structural motifs that underpin essential biological functions, including protein biosynthesis and gene expression. Understanding RNA structure is therefore fundamental to uncovering the biochemical mechanisms of life. These structures are highly dynamic and can adopt multiple conformations, which directly influence their functional roles in cellular processes.

RNA multiloops play a key role in stabilizing tertiary structures and mediating molecular interactions. Their structural diversity and variability make them particularly challenging to analyse using existing computational tools. However, the RNAloops platform has limitations in database updating and structural search capabilities. This study aims to address these gaps by modernizing the update module and implementing topology-based search mechanisms.

The proposed system increased the number of multiloops by 46% (over 40,000 new structures) through automated, repeatable updates from the PDB repository, while enabling efficient, parallelized, fault-tolerant processing and a precise, topology-based search tailored to user-defined criteria.

These improvements significantly enhance RNA structural analysis and data accessibility for researchers. The new features facilitate identification of non-redundant spatial motifs, supporting more accurate and efficient studies of RNA structure and function. The system provides a robust foundation for further development of bioinformatics tools.

RNAVIGATION – SIMPLIFYING THE WAY THROUGH DIFFERENTIAL EXPRESSION ANALYSIS

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Keywords: RNA, miRNA, differential expression analysis, DESeq2, edgeR, NOISeq, normalization, Gene Ontology, KEGG pathway, functional enrichment analysis, bioinformatics tools

RNA-seq differential expression analysis is essential for identifying molecular changes between biological conditions, but many available tools require programming skills or provide limited insight into the analytical workflow. Existing solutions often deliver results without explaining underlying logic or enabling comparison between algorithmic approaches. This creates a barrier for experimental researchers who need both accessible analysis and transparent, reproducible results.

To address this gap, we developed a user-friendly web-based platform for RNA-seq differential expression analysis. The application integrates established methods such as DESeq2 and edgeR, with planned support for NOISeq, enabling comparison across statistical models and normalization strategies. The workflow guides users through key analytical steps, explains parameters, and provides statistical summaries, including normalization and dispersion-related outputs.

To support biological interpretation, the platform includes Gene Ontology Biological Process and KEGG pathway enrichment analysis, allowing direct translation of differentially expressed gene lists into functional pathways. It also supports user-provided result tables from external analyses for merging, visualization, and further interpretation.

By combining accessible analysis, methodological transparency, functional enrichment, and article-ready visualizations, the platform bridges RNA-seq data and biological insight, empowering experimental researchers to conduct rigorous, reproducible, and interpretable transcriptomic analyses.

SECONDARY STRUCTURE CHARACTERIZATION OF HPN AND α - SYNUCLEIN BY CIRCULAR DICHROISM AND ATR-FTIR SPECTROSCOPY

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Keywords: protein aggregation, conformational changes, β-sheet formation, α-helical structure, thermal stability, temperature-induced folding

The study focused on α-synuclein and the histidine-rich protein Hpn from *Helicobacter pylori*, two proteins characterized by high structural flexibility. α-Synuclein is associated with neurodegenerative disorders, while Hpn plays an important role in nickel binding and bacterial metal homeostasis. Since changes in secondary structure may influence protein stability, activity, and aggregation behavior, the aim of the study was to compare the structural response of both proteins under different temperature conditions and identify dominant conformations.

Circular dichroism (CD) spectroscopy was used to evaluate temperature-dependent changes in secondary structure between 4 °C and 96 °C, with additional measurements at 25 °C. A complementary technique – attenuated total reflectance Fourier transform infrared (ATR-FTIR) spectroscopy, was also used to compare the obtained results describing the secondary structure at 25 °C. All spectra were recorded in phosphate-buffered saline (PBS, pH 7.2).

Based on CD measurements, Hpn showed high antiparallel β-sheet content at lower temperatures (up to ~61% at 4 °C and 25 °C), while α-synuclein exhibited a pronounced increase in α-helical content at elevated temperature (up to ~42% at 96 °C).

These findings demonstrate that temperature induces distinct conformational rearrangements in both proteins and highlight their high structural plasticity. The observed differences may be important for understanding bacterial adaptation as well as processes related to protein misfolding and neurodegeneration.

STRUCTURAL CHANGES AND AGGREGATION KINETICS OF STAPHYLOCOCCUS AUREUS PSMα1 AND δ-TOXIN

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Keywords: functional amyloids, spectroscopy, aggregation, secondary peptide structure

Amyloids are aggregates of peptides characterised by a fibrillar structure and a β-sheet secondary structure (known as cross-β). In humans amyloids have been linked to various diseases. Functional amyloids, however, are not pathological and have their functions in a healthy organism. PSMα1 and δ-toxin are bacterial functional amyloids that belong to the PSM (Phenol Soluble Modulins) peptide family. They serve as structural elements, dispersion agents~~,~~ and enhancers of virulence and assist in the formation of *Staphylococcus aureus* biofilms.

The aim of the experiment was to verify aggregation propensity and secondary structural distribution of synthetic deformylated variants of PSMα1 and δ-toxin and compare results to already existing literature.

Only PSMa1 showed the ability to change substantially its secondary structure and the propensity to aggregate. When combining the results from all used methods, it implies that PSMa1 creates β-structures when forming aggregates.

PSMα1 and δ-toxin are produced by *Staphylococcus* bacteria, including Methicillin-resistant *Staphylococcus aureus* (MRSA), which can be the cause of ~~most~~ severe infections and can even lead to sepsis. Variations in their aggregation kinetics and structure have an impact on antibiotics resistance of *S. aureus*.

STRUCTURAL DETERMINANTS OF MCPIP1 SUBSTRATE RECOGNITION REVEALED BY INTEGRATIVE RNA MODELING

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Keywords: structure modelling, structural biology, protein prediction, MCPIP1

Computational approaches have become essential for predicting biomolecular structures, particularly when experimental data remain incomplete. This is especially relevant for RNA-protein interactions, where subtle structural features often determine regulatory specificity. Understanding these determinants is crucial for elucidating mechanisms of post-transcriptional gene control.

MCPIP1 (Regnase-1) is an RNase that selectively degrades inflammatory transcripts, yet the structural basis of its substrate recognition remains insufficiently defined. To address this gap, we analyzed short RNA fragments derived from the IL-6 3'UTR-known MCPIP1 targets-using RNA Composer and RNAstructure Web Server. Six variants representing stem-loops, hairpins, and ssRNA were modeled and compared in terms of thermodynamic stability (ΔG –6.6 to +4.6 kcal/mol), loop length (3–6 nt), arm length, and the presence of guanine at the putative cleavage site.

Stable loop-containing structures with a guanine positioned within the loop-mIL-6 82-106, hIL-6 82–99, and the consensus stem-loop-exhibited features consistent with known MCPIP1 substrate preferences, whereas ssRNA fragments lacked such determinants.

These findings indicate that MCPIP1 selectivity is driven by discrete structural signatures embedded within IL-6 RNA loops, underscoring the value of combining RNA modeling with functional interpretation. This structural insight refines current models of MCPIP1-mediated mRNA decay and provides a basis for future mechanistic studies of RNA-directed immune regulation.

STRUCTURE-BASED PROTEIN FUNCTION PREDICTION WITH METAGENOMIC-DEEPFRI

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Keywords: protein function, protein structure, metagenomics, large-scale computing

Functional annotation of proteins is foundational to modern biology, translating raw sequence data into biological understanding at the scale of entire ecosystems. While sequence-based methods dominate large-scale annotation pipelines, protein structure may carry complementary information aiding in accurate function prediction. However, the computational cost of de novo structure prediction has historically restricted most pipelines to sequence-based models, leaving structural information underutilized. A problem particularly prominent in metagenomics, where datasets could contain millions of proteins of unknown origin. The recent emergence of large-scale predicted structure repositories (AlphaFold database, ESM Atlas) now offers an opportunity to incorporate structural context without prohibitive cost. Here, we introduce metagenomic-deepFRI, a framework that integrates structural templates from these repositories into functional annotation pipeline at speeds comparable to sequence-alignment methods. Integration of structural features raised deepFRI confidence scores above the default certainty threshold and increased the Information Content of predicted GO terms by up to 50%, while maintaining coverage at nearly 90% of queried proteins. By bridging high-throughput annotation with structure-informed prediction, metagenomic-deepFRI enables researchers to generate concrete functional hypotheses for uncharacterized proteins at metagenomic scale, with direct implications for environmental microbiology, biotechnology discovery, and the broader effort to map the functional dark matter of microbial communities.

SURFACE ELECTROMYOGRAPHY FOR IDENTIFYING THE EFFECT OF UNDER OR OVER-CORRECTING THE EYE'S OPTIMAL REFRACTIVE STATUS

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Keywords: electromyography, refraction, extra-ocular muscles, eye's refractive status

Recent developments in the analysis of the relations that exist between our eyes and facial muscles suggest that there are visible connections. It is possible that external factors, such as spherical over-correction applied to human eyes, could influence the activity of facial muscles.

This study focused on finding this connection between spherical over-correction of the eye and the activity of the extra-ocular muscles. The measurements of 12 subjects were completed with a special protocol designed to define the range of spherical over-correction that would produce muscle reaction. The analysis of the results showed significant differences in the medians for the high applied over-correction among the root mean square values of the signals and a significant difference for the slope for the low over-correction.

As expected, no applied over-correction did not produce any meaningful results. It has been proven, with limited confidence due to the size of the population, that these relations exist is possible that spherical over-correction applied in 0.5~D influences activity of extra-ocular muscles.

This study has proved, with limited confidence, that the relations between eye refractive status and extra-ocular muscles activity may be present and measurable with simple electromyography apparatus. This broad approach suggests, that these relations in the future may lead us into alternative ways of prescription of correction glasses.

THREE-DIMENSIONAL NUCLEAR MORPHOMETRIC ANALYSIS OF CELL NUCLEI ACROSS MOUSE TISSUES

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Keywords: nuclear morphology, chromatin textural analysis, machine learning, confocal microscopy, biological image analysis

Aberrations in nuclear architecture constitute a well-known hallmark of cancer cells, making microscopy image-based nuclear morphometric analysis a major approach in cancer diagnosis. However, changes in nuclear organization and morphology are observed not only in pathological conditions. Cell type-specific genomic programs are modulated by microenvironmental factors and closely linked to nuclear morphology and chromatin condensation states, while lineage-specific chromosome organization and increased nuclear stiffness are a characteristic of differentiated cells. Based on this, we hypothesize that pathology-derived nuclear morphometric approaches based on quantitative features of nuclear size, shape and chromatin texture can effectively distinguish between cell types originating from different mouse tissues. To the best of our knowledge, we demonstrate for the first time that a 3D SRP textural descriptor, combined with BoVW and SVM, can be effectively applied to classify cell nuclei in frozen tissue sections, and, despite distinct staining patterns, classification accuracy is comparable for images of nuclei stained with both DAPI and SYBR Green. We further identify nuclear morphological features characteristic of each tissue type, providing insights into chromatin condensation patterns as assessed by confocal microscopy, and establishing a basis for integration with genomic and transcriptomic data to link differentiation-associated nuclear remodeling with underlying molecular states.

[1] Uhler C, Shivashankar GV. Nuclear Mechanopathology and Cancer Diagnosis. Trends Cancer. 2018 Apr;4(4):320-331. doi: 10.1016/j.trecan.2018.02.009. Epub 2018 Mar 16. PMID: 29606315.
*[2] Radhakrishnan, A., Damodaran, K., Soylemezoglu, A.C. et al. Machine Learning for Nuclear Mechano-Morphometric Biomarkers in Cancer Diagnosis. Sci Rep **7**, 17946 (2017). https://doi.org/10.1038/s41598-017-17858-1*
*[3] Ďuríková, P., Šimaljaková, M. Nuclear Morphometric Analysis in Basal Cell Carcinoma: an Unrealized Potential? A Scoping Review. Bratisl. Med. J. **126**, 715–731 (2025). https://doi.org/10.1007/s44411-025-00139-z*
*[4] Rana, P., Sowmya, A., Meijering, E. et al. Estimation of three-dimensional chromatin morphology for nuclear classification and characterisation. Sci Rep **11**, 3364 (2021). https://doi.org/10.1038/s41598-021-82985-9*

TO HIDE BUT BE NOTICED: HOW GUPPY COLORATION CHANGES - A MULTI-AGENT MODEL

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Keywords: guppy, *Poecilia reticulata*, multi-agent modeling, sexual selection, predation pressure, handicap principle, maximum likelihood, Monte Carlo method

Multi-agent modeling serves as a highly effective tool for analyzing complex evolutionary and behavioral processes in animal populations. By simulating individual interactions, these models allow researchers to explore ecological dynamics that are challenging to observe directly in wild habitats.

To clarify how natural selection and sexual selection interact, this study developed a multi-agent model of guppy (*Poecilia reticulata*) populations under varying predation pressures. Parameterized with empirical data from two distinct rivers, the model investigates how male color ornamentation - specifically the number and area of black and orange spots - influences reproductive success under low and high predation risks.

The simulations revealed that while female sexual selection drives the success of highly ornamented males in low-predation environments, high predation pressure severely reduces their survival, shifting evolutionary strategies toward less conspicuous phenotypes. These findings demonstrate the utility of empirically-based agent modeling in capturing the delicate balance between sexual selection and predator avoidance.

Ultimately, this approach provides a scalable framework for predicting how environmental shifts might alter phenotypic distribution and survival strategies in diverse ecosystems.

TOWARD LIPID NANOPARTICLE-MEDIATED DELIVERY OF AM404: A LITERATURE-BASED PERSPECTIVE

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Keywords: lipid nanocarriers, AM404, drug delivery, paracetamol metabolites

Acetaminophen, broadly known as Paracetamol, has been on the market since 1955, yet its mechanism of action remains only partially understood. Recent research suggests that it is not the paracetamol molecule itself that is responsible for the drug's analgesic mechanism, but rather its metabolites, particularly AM404. This information has opened new horizons for the design and development of potent, next-generation pain-alleviating drugs. Especially useful in this context are lipid-based nanoparticles (LNPs), which can serve as an advanced platform for drug delivery, improving bioavailability and targeted delivery of the substance.

As AM404 has attracted increasing attention in recent years, there are still few studies on the design and development of LNP formulations for this molecule. This work presents a structured literature review of currently available nanocarriers suitable for molecules with similar chemical properties.

Literature findings demonstrate that molecules with chemical properties similar to AM404 yield the best results when paired with formulations such as extracellular vesicles, polymeric nanoparticles, inhalable nano-in-microparticles, and other nanoparticle systems.

The presented findings provide a strong theoretical basis for developing an effective LNP formulation for AM404 delivery, thereby creating new opportunities for personalized medicine.

TRACER: A FIRST-PASS MODEL FOR EXPLORING ALTERNATIVELY CODED GENOMES

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Keywords: Alternatively coded genomes, tRNA, codon reassignment, genome classification, machine learning, bioinformatics tool.

Alternative genetic codes challenge the universality of the canonical codon–amino acid mapping and remain poorly characterized at the genome-wide scale. Despite the increasing availability of genomic data, systematic detection of such alternations is hindered by data quality issues and the lack of scalable screening methods. Importantly, their impact on biological data analyses is potentially highly impactful and often overlooked.

Here, we introduce TRACER, a tRNA-based machine learning framework for first-pass detection of alternatively coded genomes. Using features derived from tRNA anticodon profiles, GC content, and tetranucleotide composition, TRACER enables high-throughput screening of large genomic datasets. Applied to millions of bacterial genomes, the model identified over 16,000 candidate genomes exhibiting signatures consistent with alternative coding of more than 55 genomic types. The amount and quality of produced data allowed us to distinguish biologically meaningful signals from assembly artifacts.

We demonstrate that alternative genetic coding is associated with distinct genomic signatures and follows structured, non-random patterns across genomes. TRACER provides an efficient prioritization step for much more computationally intensive tools for genetic code prediction and establishes a scalable framework for exploring genetic code variation, opening new directions for evolutionary and functional genomics.

Virtual Reality and EEG in diagnosis of hemispatial neglect

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Keywords: virtual reality, EEG, hemispatial neglect, stroke, neuroscience, signal analysis

Virtual reality (VR) is increasingly used in medicine as a tool for rehabilitation, offering controlled and immersive environments that can support patient recovery. In particular, neurological disorders such as hemispatial neglect require targeted therapies that stimulate spatial awareness and attention. Integrating VR with real-time monitoring and data collection enables more precise and adaptive therapeutic interventions.

Hemispatial neglect, often resulting from brain injury such as stroke, leads to a lack of awareness of one side of space, making rehabilitation challenging and difficult to quantify. Traditional therapeutic approaches lack precise measurement tools and real-time clinician oversight without disrupting the patient's experience. This project addresses these limitations by developing a VR-based rehabilitation system combined with a web diagnostic panel, EEG monitoring and eye-tracking module, aiming to create a measurable, interactive, and remotely supervised therapeutic environment.

The system successfully integrates a VR therapeutic application with real-time WebSocket-based monitoring, EEG and eye-tracking data collection, enabling objective assessment and remote supervision of patient rehabilitation.

This work combines immersive therapy with quantitative behavioral tracking and clinician control. The integration of eye-tracking and EEG data provides a foundation for objective evaluation of patient progress, which is often lacking in conventional therapies. The proposed architecture can be extended to other neurological conditions and may be used as a starting point for further research regarding telemedicine and VR therapies.

WhyMC - Extracting biological insights from an imaging mass cytometry foundation model

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Keywords: deep learning, explainable AI, counterfactual explanations, Imaging Mass Cytometry, multiplex imaging, tumor immune microenvironment

Multiplex imaging allows researchers to create detailed spatial maps of the tumor microenvironment, serving to further our understanding of the biological and clinical aspects of cancer. While deep learning models excel at extracting complex patterns from this data, their lack of interpretability often limits their reliability in biological research. Using ImmuVis, a foundation model capable of virtual staining - predicting the spatial expression of an unknown marker given a set of input markers, we aim to discover the biological meaning of those predictions. We propose WhyMC, an interpretability framework that uses counterfactual explanations to quantify how changes to the input markers impact the predictions. Using this method we explore the expression landscape of PD-L1, a known prognostic marker for patient response to immunotherapy. By revealing the specific perturbations influencing the models predictions, this approach expands our biological understanding of the tumor microenvironment by uncovering less obvious spatial patterns. Furthermore, the ability to explain each prediction is necessary for such models to safely be deployed in a clinical setting.

XAI ANALYSIS OF MICROBE CLASSIFICATION ON THE DIBAS DATASET

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Keywords: convolutional neural networks, segmentation-based approaches

Computer vision models offer many advancements in microbiology, such as streamlined identification of microbes from microscopic images. However, to ensure these technologies are reliable for broader deployment, it is critical to evaluate exactly how convolutional neural network (CNN) models process and interpret biological data.

Although CNNs achieve high classification accuracy on datasets like DIBaS, quantitative metrics alone do not guarantee that a model has learned meaningful features. Deep learning architectures are highly susceptible to shortcut learning, a process where the network exploits spurious correlations — such as lighting artifacts or image noise — rather than recognizing actual microbe morphology.

Model analysis through XAI techniques reveals that while the classification model achieved ~95% accuracy, it relies mainly on shortcut learning to make its predictions. This suggests that it failed to learn robust, generalizable features from the provided data, and would likely underperform in real-world scenarios.

These findings highlight an important limitation in evaluating microbiology models, demonstrating that high accuracy can sometimes obscure a model's reliance on non-biological artifacts. As a result, this study supports the use of Explainable AI (XAI) as a supplementary validation tool to better assess true diagnostic performance. Future research should focus on developing training strategies that mitigate shortcut learning, such as segmentation-based approaches.

Bioinformatic Analysis of Foldamers' and Miniproteins' Functional and Structural Properties

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Proteins and synthetic protein-like molecules play essential roles in biological systems. Bioinformatic analyses enable the prediction of structural organization, stability and physicochemical properties of peptides and engineered biomolecules, supporting the understanding of their functions and potential applications.

Previous studies have shown that coiled-coil peptides containing trans-aminocyclopentanecarboxylic acid (trans-ACPC) incorporated into their sequences had more stable helical structures and were less resistant to various factors [1]. Proline residues are known to bend α-helical structures through changes in peptide chain conformation. The aim of this study was to evaluate the influence of the substitution of trans-ACPC with proline residues in amino acid sequences on peptide organization, stability, and tendency to aggregate.

Based on structural and physicochemical analyses, peptides containing proline residues were less stable and showed a lower tendency to aggregate compared with analogues containing trans-ACPC, alanine, or leucine residues.

These results showed that even small differences in the amino acid sequences of peptides can cause significant changes in their structural and physicochemical properties. Such analyses may support the evaluation of peptide folding behavior and stability before experimental validation. Understanding the structure and properties of proteins, as well as their synthetic analogs can help predict their functions and identify potential applications, including in medicine and drug design.

References:

[1] Szulc N, Wojtas M, Kral T, Pokorná Š, Hof M, Szefczyk M. Solvent-Encoded Intrinsic Emission and Self-Assembly of Coiled-Coil-Based Foldamers. J Phys Chem B. 2026 Jan 29;130(4):1447-1459. doi: 10.1021/acs.jpcb.5c08320. Epub 2026 Jan 18. PMID: 41549507.