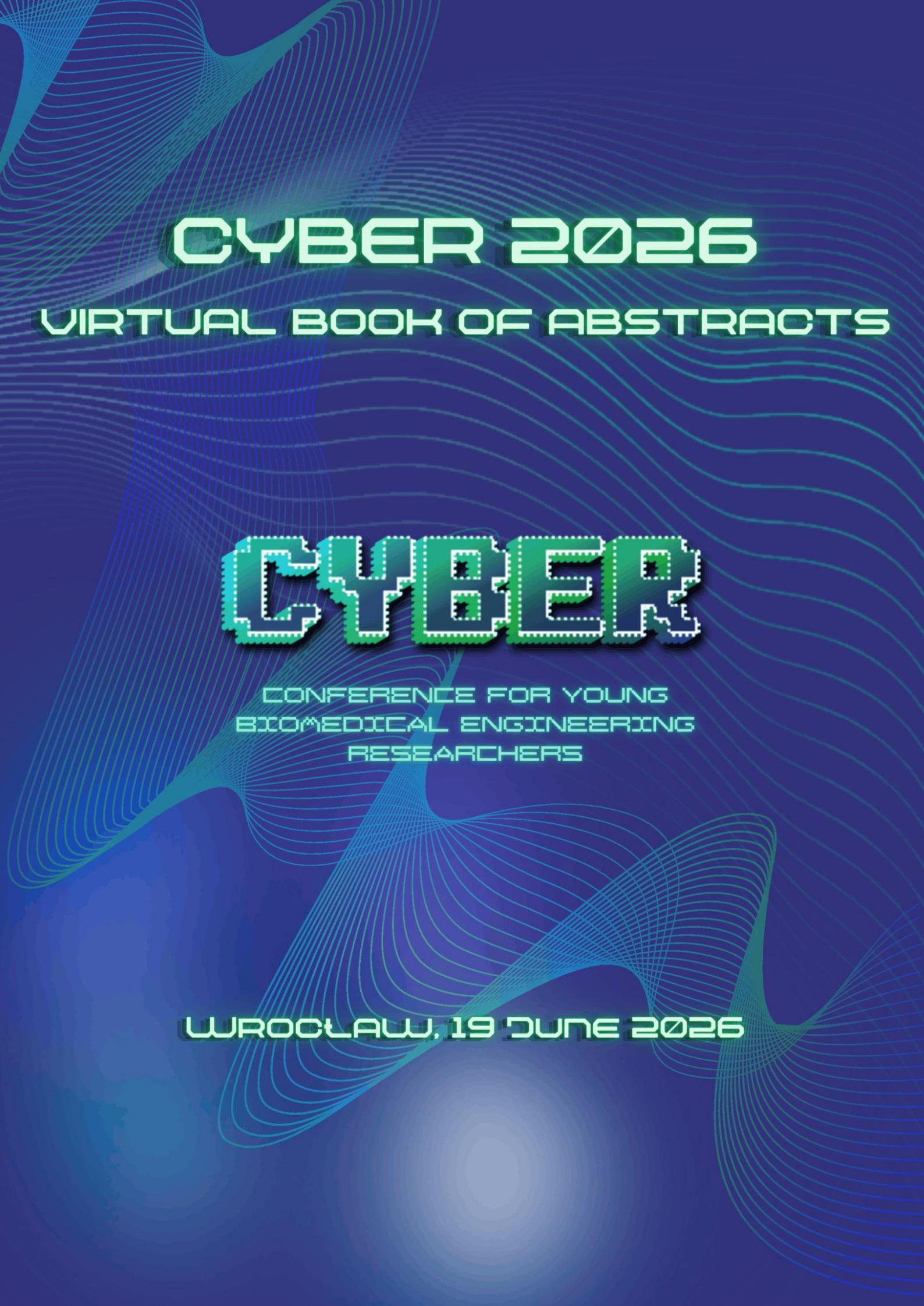




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ORAL PRESENTATIONS

What can MEG signals tell us about the hidden architecture of the human auditory cortex?

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Keywords: auditory cortex, computational modelling, connectivity, event-related fields, evolutionary algorithms

Abstract

Background: Unravelling the structural organisation of the human auditory cortex (AC) remains a significant challenge. Because invasive histological mapping is not ethically possible in humans, current models of human AC are extrapolated from animal data. While non-invasive methods like magnetoencephalography (MEG) provide insight into human AC dynamics, they lack the resolution to distinguish between individual cortical fields. Interpreting MEG signals is difficult because they reflect the combined activity of large populations of neurons and are often affected by a low signal-to-noise ratio. This creates a gap in auditory neuroscience: we can record MEG signals, but we cannot easily 'see' the latent network architecture that generates them. Our work addresses this gap by demonstrating that the temporal morphology of these signals holds recoverable information about the hidden connectivity.

Materials and Methods: We used a computational AC model with 13 distinct auditory fields, organised into a core-belt-parabelt hierarchy, capable of generating in-silico MEG signals. Using this architecture, we designed and implemented an evolutionary algorithm (EA) to estimate connection weights between the fields. The optimisation aimed to maximise alignment between in-silico MEG signals and in-vivo human MEG data. To ensure robust statistical inference, our research used leave-one-out cross-validation and a custom anomaly-detection procedure based on Extended Isolation Forests to identify outliers in the high-dimensional parameter space. The entire framework was applied to two independent MEG datasets.

Results: The EA successfully improved the AC model performance. The mean normalised fitness function (a measure of model accuracy) increased from 0.673 ± 0.119 to 0.909 ± 0.037 in Dataset A. In Dataset B, it rose from 0.568 ± 0.105 to 0.879 ± 0.041 . Applying this framework across two independent datasets identified consistent connectivity patterns. Statistical analysis of the inferred parameters, using the false discovery rate (FDR) correction, revealed a significant dominance of corticothalamic feedback over thalamocortical feedforward projections. In the left hemisphere, belt-to-core feedback exceeded core-to-belt feedforward projections, while interactions within the belt were mainly feedforward.

Conclusion: Our results demonstrate that MEG morphology contains recoverable information regarding connectivity patterns in the human AC. By combining computational modelling, in-vivo MEG data, and optimisation, this approach provides a non-invasive means of inferring latent features of AC organisation. Our structural findings suggest that the human auditory system does not rely on a simple one-way pathway. Instead, higher-level areas send strong feedback to actively shape earlier stages of sound processing.

Selective RNA-Based Progerin Silencing for Hutchinson–Gilford Progeria Syndrome Therapy

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Keywords: small interfering RNA, RNA-interference, gene therapy, progeria, genetic disorder.

Abstract

Hutchinson–Gilford progeria syndrome (HGPS) is a rare fatal genetic disorder caused by a *de novo* point mutation in the *LMNA* gene, which encodes the nuclear structural proteins lamin A and lamin C that also play an important regulatory role. Patients with HGPS show symptoms of premature aging and usually die at around 14 years of age due to cardiovascular disease. The mutation activates a cryptic splice site, leading to the production of a truncated form of lamin A known as progerin. In contrast to lamin A, progerin retains a C-terminal farnesyl group because it cannot undergo complete post-translational processing. This modification results in permanent anchoring of progerin to the inner nuclear membrane. Accumulation of progerin disrupts nuclear architecture, alters chromatin organization and gene expression. Currently, the only approved therapy is lonafarnib – a farnesyltransferase inhibitor that slows disease progression after prolonged administration [1]. However, it does not fully restore cellular function nor eliminate disease manifestations, highlighting the need for strategies that directly silence progerin production.

The aim of the study was to achieve selective suppression of progerin using siRNAs designed to recognize mutated splice site in progerin mRNA. For the screening we established a cellular platform based on HeLa cells stably expressing GFP-lamin A or GFP-progerin, enabling quantitative assessment of protein levels via fluorescence-based assays. SiRNA candidates were designed and evaluated for both efficacy and specificity. The best sequences achieved strong and selective reduction of GFP-progerin without affecting GFP-lamin A level [2, 3]. Next chemically modified siRNA variants were generated to enhance nuclease resistance and improve *in vivo* applicability, as confirmed by stability assays in mouse serum. Selected siRNAs were subsequently validated in fibroblasts derived from HGPS patients. Western blot analysis confirmed a pronounced decrease in progerin protein level, with no detectable changes in lamin A or lamin C expression.

While the current work focuses on synthetic siRNA delivery, future directions may include vector-based expression systems such as shRNA or miRNA constructs to enable sustained gene silencing *in vivo*. Overall, our results support siRNA-mediated targeting of progerin as a promising and precise therapeutic strategy for HGPS that may complement or extend the benefits of current treatments such as lonafarnib.

Acknowledgments

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Brain-Age Estimation from Electroencephalography (EEG) and Functional Near-Infrared Spectroscopy (fNIRS) in Adult Populations: A Scoping Review

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Keywords: EEG, fNIRS, brain ageing, brain age gap, brain age estimation, deep learning

Abstract

Introduction. Brain age is an established neuroimaging biomarker [1], with the brain age gap linked to neurodegenerative progression [2]. Magnetic Resonance Imaging (MRI) models achieve Mean Absolute Error (MAE) of 2–6 years [3], EEG and fNIRS could support lower-cost, out-of-hospital assessment. This review maps adult EEG and fNIRS brain-age studies by architecture, performance, and bias correction.

Research question. This scoping review asked three research questions (RQ): architectures and performance for adult EEG/fNIRS brain-age estimation (RQ1); evidence and gaps for integrated EEG–fNIRS estimation (RQ2); and regression-toward-the-mean correction (RQ3).

Methodology. Following PRISMA-ScR, five databases were searched for 2016–2026 records using “brain age” AND EEG/fNIRS terms, supplemented by 22 manual results. Eligible studies were original adult EEG- or fNIRS-based brain-age/ageing studies with quantitative performance. Exclusions covered paediatric-only, other modalities, non-ageing topics, non-original, and non-English papers. From 396 records, 246 remained after deduplication, 79 after abstract screening, and 28 after full-text review.

Findings. Of 79 studies, 27 reported continuous brain-age regression (MAE or RMSE), one binary classification, and the rest R2, accuracy, or design-stage proposals. Classical ML and deep learning were roughly balanced.

Table 1. Brain-age regression studies by modality and architecture.

Modality	Architecture class	N studies	MAE range (years)	RMSE range (years)	Bias correction
EEG	Classical ML	14	4,42 – 15,54	3,29 – 11,96	Mixed
EEG	Deep learning	12	2,645 – 15,99	3,327 – 15,1	Mixed
fNIRS	Classical ML	2	-	8,77 – 9,06	Not reported
fNIRS	Deep learning	0	-	-	-
EEG + fNIRS	Any	0	-	-	-

EEG MAE spanned 2.645–15.99 years, highly heterogeneous. No fNIRS study achieved valid continuous regression: Ji et al. [4] found near-zero or negative correlations, and Ilvesmäki et al. [5] used only binary classification. Bias correction (RQ3) was inconsistent: of 26 regression studies, most reported uncorrected and only two corrected metrics.

Knowledge gaps (RQ2). No included study estimated continuous brain age using fused EEG–fNIRS data. The only public simultaneous EEG–NIRS dataset [6] lacks brain-age labels, making it the main methodological gap.

Perspectives. Three gaps emerge: inconsistent EEG bias correction, absent fNIRS continuous regression, and no EEG–fNIRS integration. The planned contribution: a synchronised multimodal deep-learning estimator with multiple fusion strategies and regression-toward-the-mean correction.

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Design and Implementation of a Low-Cost, 6-Channel sEMG System for Bionic Limb Control

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Keywords: electromyography, biosignal processing, embedded systems, instrumentation amplifiers, wireless data transmission

Abstract

The subject of this work is the development and optimization of a low-cost, wireless, six-channel surface electromyography (sEMG) acquisition platform designed for real-time muscle activity monitoring. In accordance with medical device safety standards, the hardware is engineered as a type BF (Body Floating) applied part, utilizing battery power to ensure electrical isolation from the main grid. The architecture is based on an ESP32 microcontroller, operational amplifiers, and active analog filtering stages configured to a passband of 16 to 480 Hz.

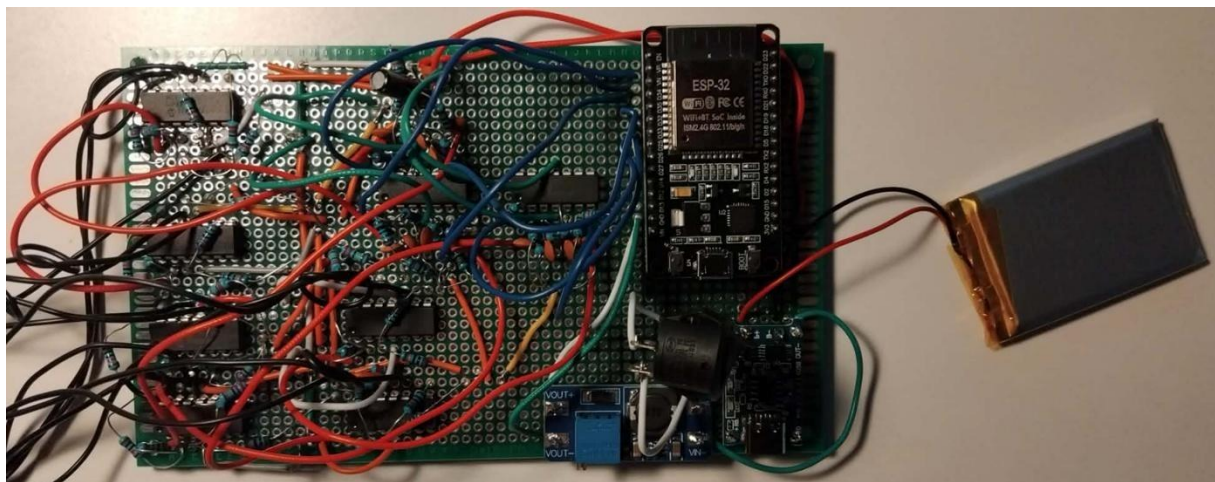


Fig. 1 Developed 6-channel sEMG acquisition hardware based on an ESP32 microcontroller and a multi-channel MCP6004 analog front-end.

A major engineering challenge addressed in this project is maintaining signal integrity under intense electromagnetic interference caused by the onboard Wi-Fi module pulsing during UDP data transmission. To provide strong attenuation of these high-frequency disturbances, a virtual ground stabilization circuit was introduced into the power management topology. The software layer utilizing User Datagram Protocol (UDP) is designed to stream raw 1000 Hz data channels to a Python-based visualization tool. The current stage of development demonstrates the stabilization of the analog front-end noise floor, establishing a solid baseline for the forthcoming implementation and comparative validation of various digital signal processing and feature extraction methods intended to optimize classification accuracy and latency for active upper-limb prosthetic control.

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Shared-clock synchronization of independent EEG and video streams for a wireless outpatient video-EEG system

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Keywords: video-EEG, Lab Streaming Layer, ambulatory monitoring, multimodal synchronization, epilepsy

Abstract

Long-term video-electroencephalography (video-EEG) is the diagnostic standard for distinguishing epileptic from non-epileptic events and for characterising seizure semiology, with minimum standards for inpatient monitoring formalised by the ILAE and IFCN [1]. Hospital-based monitoring units are nonetheless constrained by bed availability, cost and patient waiting times, motivating a sustained effort to bring diagnostic video-EEG into the home through supervised, ambulatory and cloud-based telemetry [2]; sub-frame-accurate synchronisation of independent wireless sensor streams over a consumer-grade network remains a core engineering hurdle in this setting.

A prototype addressing this hurdle is presented. Two Raspberry Pi nodes — a Zero 2W acquiring EEG over USB from a BrainTech Perun32 amplifier, and a 3B+ producing hardware-encoded H.264 from a Pi Camera module — publish independent Lab Streaming Layer (LSL) outlets onto a shared logical clock. Synchronisation is provided entirely by per-sample LSL timestamps and periodic clock-offset queries, exploiting the software-only, zero-configuration framework introduced for multimodal neurophysiological recording [3]. A workstation acts as the LSL consumer, recording both streams together with their offset history into a single session. The approach builds directly on the open-source, millisecond-synchronised video-EEG system of Raghavan et al. [4], extending it from a wired laboratory configuration to two independently networked wireless sensor nodes operating on commodity hardware.

Synchronisation accuracy is to be validated with a hardware reference marker — a microcontroller-driven LED in the camera's field of view fired simultaneously with a TTL pulse into the amplifier's dedicated hardware synchronization input (Mini-DIN 8, RIN1) — providing a ground-truth temporal offset and a measurement of drift across multi-hour recordings. The system is designed to achieve milliseconds-scale alignment between the two modalities, and continuous operation has been verified over multi-hour runs.

Future work will extend the platform with on-device classification for ambulatory seizure detection and a paired alarm that, on detected ictal onset, prompts the patient through a short standardised battery of responsiveness, orientation and language items, recorded synchronously with the EEG and video so that the ictal testing routinely performed in inpatient monitoring units can be replicated in the outpatient setting.

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14-3-3 proteins as partners of NPAS4, a bHLH-PAS family member

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Keywords: 14-3-3 proteins, NPAS4, bHLH-PAS, protein-protein interactions, neurodegeneration

Abstract

14-3-3 proteins are highly expressed throughout the body and implicated in many diseases, from cancer to neurodegenerative disorders. These proteins belong to a family of homologous proteins existing in seven different isoforms (β , γ , ϵ , η , ζ , σ , and τ/θ) involved in many cellular signalling pathways via protein-protein interactions (PPI). In mammals, their highest expression has been observed in the brain. NPAS4 (Neuronal PAS domain-containing protein 4), functioning as a neuroprotective factor, belongs to the basic helix-loop-helix-Per-ARNT-Sim (bHLH-PAS) family of transcription factors. The bHLH-PAS transcription factors play a significant role as crucial sensors of environmental and cellular signals, with their activity tightly regulated by nucleocytoplasmic shuttling. Some members of the bHLH family were shown as partners of 14-3-3 proteins, which influence their localization and activity. To date, no data has shown whether NPAS4 interacts with 14-3-3 proteins, though such interaction would be important for understanding complex pathways of neurodegeneration development involving Tau (microtubule-associated protein). The aim of this study is to test the hypothesis concerning the interaction between 14-3-3 and NPAS4. To predict putative 14-3-3 binding sites in NPAS4, we performed in silico analysis using Scansite 4.0 and ELM. Interestingly, the predicted motifs were found within intrinsically disordered regions (IDRs). For preliminary verification, we performed co-localization studies of NPAS4 and 14-3-3 in neuronal cells using confocal microscopy. Our analysis showed that fluorescently tagged NPAS4 and 14-3-3 co-localize in transfected N2a cells, supporting a possible interaction between these proteins. The findings suggest that 14-3-3 proteins may regulate NPAS4 subcellular localization and activity. Interaction will be studied further in living neuronal cells using pull-down assays. To test the structural basis of 14-3-3-NPAS4 interaction, we will use purified recombinant proteins. We were able for the first time to obtain full-length NPAS4 expression in *Pichia pastoris*. Further experiments are needed to optimize the purification procedure of NPAS4 and 14-3-3.

Silicone Coatings With Carbon Nanotube-Induced Nanotopography for Biofouling Control

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Keywords: carbon nanotubes, silicone coatings, nanotopography, bacteria, biofouling

Abstract

Biofouling, which involves the adhesion and proliferation of microorganisms on material surfaces, is a significant issue in biomedical and industrial systems, especially in silicone-based devices that are susceptible to bacterial colonisation. This study developed silicone coatings with controlled nanotopography, induced by multi-walled carbon nanotubes (MWCNTs), as a passive strategy to reduce microbial adhesion. The coatings were fabricated using a poly(dimethylsiloxane) matrix modified with MWCNTs of various outer diameters (6–13 nm, 50–90 nm and 110–170 nm), which were then deposited onto glass and stainless steel substrates.

The influence of nanotube diameter on coating morphology, surface wettability, bacterial adhesion, metabolic activity, coating stability and haemocompatibility was systematically investigated. Surface nanotopography and morphology were characterised using scanning electron microscopy (SEM), while quantitative roughness analysis was performed using profilometry. Wettability was assessed through static contact angle measurements. SEM observations and profilometric analysis confirmed the formation of hierarchical micro- and nanoscale surface structures, with nanotube diameter being found to strongly influence coating topography. The incorporation of MWCNTs significantly increased surface hydrophobicity, with contact angle values reaching approximately 130–150°, depending on nanotube diameter and substrate type. Coatings modified with 110–170 nm MWCNTs exhibited the highest contact angles and the most pronounced nanotopographical features. The antibiofouling performance of the coatings was evaluated using *Staphylococcus aureus* and *Escherichia coli* under static-dynamic incubation conditions. Bacterial adhesion and viability were assessed using optical density measurements, colony-forming unit (CFU) analysis and optical coherence tomography (OCT), which enabled visualisation of surface-associated bacterial structures. MWCNT-modified coatings significantly reduced bacterial adhesion and biofilm-associated growth compared to unmodified silicone coatings. The strongest effect was observed for coatings containing 110–170 nm MWCNTs, achieving bacterial growth inhibition of up to 67.1% for *S. aureus* and 42.5% for *E. coli*. OCT cross-sectional imaging confirmed the absence of stable bacterial structures and biofilm-like organisation on nanotube-modified surfaces. In contrast, well-developed structures were observed on control and silicone-coated substrates. The effect of nanotubes on bacterial metabolic activity was investigated using a resazurin assay combined with absorbance and fluorescence spectral analysis. This revealed a reduction in bacterial metabolic response that was dependent on the concentration of MWCNTs present. Furthermore, coating eluates showed no detectable nanotube release under dynamic conditions, and haemolysis remained below 2% for all coating variants, indicating good haemocompatibility.

These results demonstrate that nanotopography induced by MWCNTs is a promising strategy for developing durable, stable and biocompatible antibiofouling silicone coatings with potential applications in biomedical devices and industrial systems requiring controlled microbial adhesion.

Post-Implantation ROS Drivers to Guide Antioxidant Cardiovascular Implant Design

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Keywords: oxidative stress, vascular cells, restenosis, intravascular implant

Abstract

Restenosis remains a major complication following percutaneous coronary intervention [1]. Post-implantation vascular injury triggers an inflammatory response, where reactive oxygen species (ROS) generation and oxidative stress in vascular cells accelerate neointimal hyperplasia [2]. Understanding these specific triggers is crucial for developing effective antioxidant implant coatings. This study investigated the capacity of specific proinflammatory and oxidative stimuli to initiate abrupt ROS generation in vascular endothelial cells. Human Umbilical Vein Endothelial Cells (HUVECs) were exposed to physiological proinflammatory stimuli encountered post-implantation: tumor necrosis factor α (TNF α) and oxidized phospholipids (OxPAPC), alongside known ROS inducers: Lipopolysaccharide (LPS) and tert-butyl hydroperoxide (TBHP). Intracellular ROS generation was quantified using a cell permeant reagent 2',7' –dichlorofluorescein diacetate (DCFDA). Lactate dehydrogenase and Cell Counting Kit-8 assays were performed in parallel to validate cell viability following dye loading and acute treatment. Under non-toxic conditions, OxPAPC and TBHP were identified as the most potent drivers of acute oxidative stress in HUVECs. Consequently, antioxidant molecule screening should focus specifically on scavenging OxPAPC-induced radicals to effectively attenuate post-implant inflammation. Functionalizing cardiovascular implants with these targeted antioxidant molecules represents a promising therapeutic strategy to mitigate localized ROS generation and prevent restenosis.

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Bacterial Hpn protein as a potential modulator of A β aggregation in Alzheimer's disease

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Keywords: amyloids, humane microbiome, *Helicobacter pylori*, histidine-rich protein

Abstract

Amyloids are highly ordered fibrillar aggregates with a characteristic cross- β -sheet structure formed during protein and peptide misfolding [1]. Their accumulation is a hallmark of neurodegenerative disorders, including Alzheimer's disease (AD), which is associated with the aggregation of β -amyloid (A β) peptides and tau protein. Aggregation-prone proteins can also be produced by bacteria. One example is *Helicobacter pylori* – a gastric pathogen responsible for peptic ulcer disease, which secretes the Hpn protein.

Hpn is unusual due to its high hydrophilicity and exceptionally high histidine content (~47%), distinguishing it from typical hydrophobic aggregation-prone proteins. Recombinant Hpn has previously been shown to form amyloid-like fibrils [2]. In contrast, our recent studies demonstrated that synthetic Hpn predominantly forms irregular aggregates. We also identified two aggregation-prone regions (APRs), Hpn(11–37) and Hpn(4–38), which may also be classified as cryptic amyloidogenic regions (CARs) [3]. Their amyloidogenic potential is likely masked within the full-length protein sequence. In full-length Hpn, disulfide bond formation at the C-terminus and the presence of a structural turn probably inhibit fibril formation.

Recent studies indicate a possible association between AD and *H. pylori* infection [4]. Moreover, *in vitro* studies indicate that Hpn can cross the blood-brain barrier [4][5], while the gut-brain axis may provide an additional route for interactions between Hpn and A β peptides. Such interactions could enhance amyloid aggregation and plaque formation, potentially accelerating AD progression.

The main aim of my doctoral research is to investigate the interactions between Hpn, its identified APRs/CARs, and A β peptides using a combination of experimental techniques, including electron microscopy (EM), thioflavin T (ThT) fluorescence assays, Fourier-transform infrared (FTIR), and circular dichroism (CD) spectroscopies [1][6]. Our results indicate that full-length Hpn inhibits A β aggregation, whereas the identified APRs/CARs accelerate this process. These findings may provide new insights into the role of *H. pylori* in AD pathogenesis and support the identification of novel therapeutic targets.

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Amelogenin – a model biomolecule for investigating properties and pathways of self-assembling proteins

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Keywords: amelogenin, aggregation-prone regions, amyloids, aggregation, intrinsically disordered proteins

Abstract

The majority of proteins contain at least one domain that lacks a well-defined structure and is instead spatially flexible and intrinsically disordered [1]. These fragments can drive pathogenic or functional protein aggregation, leading to the emergence of amyloid fibrils as well as amorphous or circular aggregates. Specific sequential and structural properties determining the final protein complex architecture and its pathogenic potential remain unclear. In this study, we address this gap using amelogenin as a model protein exhibiting diverse aggregative behaviors depending on isoform length and amino acid composition. This approach may help elucidate how molecular features determine the final aggregate characteristics. The analysis was performed on amelogenin isoforms h174, h146, and TRAP reported by de Sousa et al. [2], which were subjected to bioinformatic analysis and compared with their described behavior.

Multiple sequence-based amyloidogenicity predictors showed partial agreement in identifying the region GYINFSYEVLTPLKQYQSIR as aggregation-prone. This was supported by AlphaFold Server predictions for hexamers of each isoform, indicating β -sheet formation involving this region. Reported AFM images of h146 and h174 show, that they form amyloid-like fibrils with distinct morphologies: h146 produces more condensed fibrils and h174 forms branched, loosely organized networks, possibly due to the additional hydrophilic C-terminal region reducing fibril compaction. In contrast, TRAP, which contains the amyloidogenic sequence but lacks both the central hydrophobic domain and the C-terminal region, does not form fibrils and instead assembles into small circular structures. Structural models generated with the AlphaFold Server suggest that in TRAP multimers the amyloidogenic region may be partially buried due to a local bend, whereas in h146 and h174 the corresponding segment appears more extended and solvent-exposed, potentially increasing its accessibility for intermolecular interactions. In this context, the central hydrophobic domain may contribute to a structural arrangement that exposes the aggregation-prone region, enabling the effective bonding between molecules. Further analysis allowed to define specific features possibly governing non-pathological characteristics of amelogenin fibrils. As stated in de Sousa et al., amelogenin fibrillation can be regulated by proteolysis, leading to non-aggregating products. The results from the SAPS tool [3] confirmed the presence of the polar C-terminal region, which may reduce fibril compactness. The amino acid composition shows that the central domain is proline-rich, which may destabilize fibrils and increase structural flexibility.

These findings may contribute to a better understanding of how specific sequence features regulate self-assembly in intrinsically disordered proteins, and highlight characteristics that may serve as indicators of distinct aggregation pathways in other proteins. Such insights could also support future studies aimed at predicting aggregation behavior in biological and biomaterial contexts.

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From MRI to ECG – tissue polarization model

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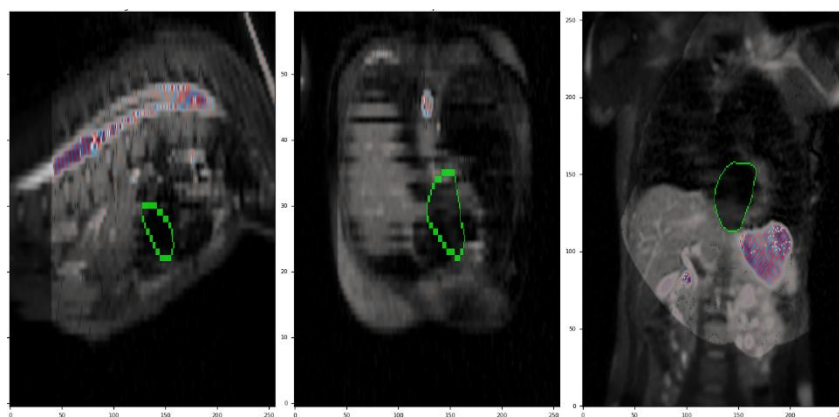
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Keywords: mri, ecg, anisotropic, propagation, model, simulation, polarization, medical, imaging, ECGi

Abstract

One of new and interesting methods in medical imaging is ECGi. It allows to reconstruct heart electrical activity from 12 lead ECG. From the clinician standpoint it's useful but shouldn't be treated as a source of ground truth [1]. Buchner's Molecular theory of Biopotentials predicts that voltage applied to tissue generates local ionic currents [2]. The resulting disturbance is transmitted at a finite rate [3] via displacement currents that do not require the flow of charge carriers [4]. Thus, we propose an anisotropic biopotential model based on forementioned assumptions. Our goal is to model potential pathways from pericardium up to skin surface and therefore bind heart to skin regions. Which could increase spatial resolutions of such techniques as ECGi. Claiming water as dominating factor of tissue polarization we use t2-weighted, fat saturated MRI images to simulate disturbances (figure 1).



As verification we use electrical activity isochrones from EDGAR database paired with body surface potential maps (BSPM). Model is currently under development, but early findings correlate with different scientists who studied influence of food intake on ECG [5].

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Digital Tracking and Quantitative Analysis of Endothelial Cell Migration under Proinflammatory Conditions

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Keywords: endothelial dysfunction, inflammation, cell migration, cardiovascular disease

Abstract

The vascular endothelium plays a crucial role in maintaining vascular homeostasis, regulating inflammatory responses, and supporting regeneration of the vascular wall [1]. Endothelial cell migration is one of the key mechanisms responsible for preserving endothelial integrity and proper vascular function. Disturbances in this process are closely associated with chronic inflammation and the development of cardiovascular diseases, particularly atherosclerosis. Oxidized low-density lipoprotein (oxLDL), recognized as an important proinflammatory mediator, contributes to endothelial dysfunction through the induction of oxidative stress and activation of inflammatory signaling pathways [2, 3].

The main aim of this study was to analyze the influence of oxLDL on endothelial cell migration parameters under *in vitro* conditions. Human umbilical vein endothelial cells (HUVECs) were cultured and divided into a control group and an experimental group exposed to oxLDL at a concentration of 50 µg/mL. Cell migration was recorded using time-lapse microscopy with the Celloger Nano system during a 12-hour observation period with 5-minute acquisition intervals. The obtained image sequences were analyzed using *ImageJ* software with the *Manual Tracking* plugin, while migration trajectories and quantitative migration parameters were further evaluated using the *Chemotaxis and Migration Tool*.

The analyzed parameters included migration velocity, accumulated distance, Euclidean distance and directionality. Statistical analysis ($\alpha = 0.05$) revealed that exposure of HUVECs to oxLDL significantly increased migration velocity (0.58 ± 0.08 vs. 1.34 ± 0.21 µm/min) and accumulated distance (420.54 ± 57.94 vs. 963.75 ± 154.05 µm) compared with the control group, indicating enhanced overall motility of endothelial cells. Simultaneously, a significant decrease in directionality (0.18 ± 0.09 vs. 0.10 ± 0.07) was observed, indicating impaired coordination and spatial organization of migration trajectories. These findings suggest that oxLDL primarily induces chemokinetic rather than chemotactic responses, resulting in increased but less efficient endothelial cell migration.

In conclusion, the study demonstrated that oxLDL significantly alters endothelial cell migration by increasing cell motility while disrupting the coordination, organization, and directionality of migration trajectories. These changes may impair mechanisms responsible for vascular repair and endothelial regeneration. From both biological and clinical perspectives, the obtained findings improve the understanding of endothelial dysfunction under inflammatory conditions and may support the development of future therapeutic strategies targeting vascular regeneration, endothelial repair and cardiovascular diseases associated with chronic inflammation, including atherosclerosis and complications following vascular interventions such as angioplasty and stent implantation.

Acknowledgments

This study was conducted as part of a Master's thesis supervised by Przemysław Sareło, MD, PhD, Eng.

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Evaluation of the Clinical Applicability of Deep Learning-Based Tool for Meibomian Glands Analysis

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Keywords: meibomian gland dysfunction, deep learning, dry eye disease

Abstract

The main aim of this study was to evaluate the clinical applicability of a previously proposed deep learning tool (DLT) [1] for automatic analysis of meibomian gland (MG) features and to assess its versatility in analyzing images from different devices. Secondary aim was to determine whether different eyelid eversion conditions affect automatic segmentation. The final aim was to propose a direct conversion of the percentage of MG loss assessed by the DLT into subjective grading scales commonly used in clinical practice: 4-grade Arita and 5-grade Pult scales. DLT was originally trained using images from Oculus Keratograph 5M (K5M). In this study DLT was evaluated on separate image datasets from K5M and two additional devices: Medmont Meridia (MD) and Topcon SL-D701 (TPC). Study included data from 54 subjects. For each patient, two high-quality images of the upper and lower eyelids were taken, suitable for automatic analysis, meaning they were in focus, well-centered, and fully everted. Consequently, 39 lower and 39 upper eyelid images per device were included for automatic segmentation. Results were verified, errors classified and manual correction was made when necessary. The effect of correction was evaluated by comparing automatically computed MG features, such as length, width, and loss, before and after correction, using a paired t-test or Wilcoxon signed-rank test. The agreement between paired images was analyzed using intraclass correlation coefficients (ICC). A separate dataset of 167 images of different eyelids, captured with K5M or MD, was used to optimize the MG loss percentage thresholds for automatic assignments of Arita and Pult grades. An iterative grid search was performed with a step size of 1% to maximize the quadratic weighted Cohen's kappa coefficient (κ) against expert subjective assessment. Quantitative analysis revealed that the highest rate of corrections was observed in the lower eyelids for TPC: 24%, primarily due to tarsus annotation errors, compared to 10–15% for the K5M and MD, where errors were mainly caused by gland omission or false-positive annotations. Significant differences between automatic and corrected annotations were found for lower eyelid in MG loss: K5M $8.1 \pm 7.1\%$ ($p=0.018$), MD $4.9 \pm 2.5\%$ ($p=0.003$), TPC $14.7 \pm 18.2\%$ ($p=0.005$). Inter-eversion agreement was good for upper and moderate for lower eyelid. TPC showed the lowest reliability of MG loss assessment for lower eyelid ($ICC=0.43$), with the same mean difference as K5M: $10 \pm 10\%$. A threshold of 23% loss was established as a cutoff for the absence of MG loss (Grade 0 in both scales). Optimized thresholds for Arita: Grade 1: 23–40%; Grade 2: >40% and Pult: Grade 1: 23%–33%, Grade 2: 34%–50%, Grade 3: >50%, achieved high agreement with expert grades ($\kappa=0.78$, $\kappa=0.74$, respectively). In conclusion, the segmentation results for TPC images require the greatest expert supervision, likely due to uneven target illumination, which causes peripheral underexposure of the eyelid. Small lower eyelid tarsus area makes DLT analysis more sensitive to errors. Nevertheless, the DLT provides reliable automatic evaluation of MG morphology regardless of the device used and eyelid eversion conditions. Specialist supervision remains essential for abnormal glands or when the eyelid is difficult to evert. The proposed thresholds require further optimization but show potential for automatic Arita and Pult grading in clinical practice.

Acknowledgments

The study was supported by the National Science Center, Poland, SONATA BIS grant 2021/42/E/ST7/00345.

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Speckle Noise Analysis in Corneal OCT Imaging for Early Detection of Forme Fruste Keratoconus

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Keywords: corneal microstructure, keratoconus, speckle noise, optical coherence tomography

Abstract

Keratoconus is a progressive, non-inflammatory corneal ectasia leading to corneal thinning, irregular astigmatism, deterioration of visual quality and, in severe cases, to the necessity of corneal transplantation. Early diagnosis of the disease remains a significant clinical challenge, particularly in its subclinical form known as forme fruste keratoconus (FFK) [1]. It presents no unambiguous clinical symptoms and remains undetectable by conventional diagnostic tools, making early intervention difficult to implement in a timely manner. Recent advances in anterior segment imaging and image-processing techniques have increased interest in the diagnostic potential of optical coherence tomography (OCT) [2]. Particular attention has been directed toward speckle noise analysis. Speckle noise, a characteristic interference pattern appearing on OCT images because of coherent light scattering, has generally been regarded as an imaging artefact. However, recent studies suggest that it contains valuable information related to tissue microstructure and light-scattering properties of the cornea [3]–[6]. The study investigates whether the analysis of speckle patterns visible in corneal OCT images can serve as a potential tool for early detection of FFK. The main research hypothesis assumes that quantitative analysis of OCT speckle characteristics may enable identification of microstructural corneal alterations before clinical manifestations of keratoconus become detectable using standard diagnostic methods. The proposed methodology includes acquisition of anterior segment OCT images from healthy subjects, patients with manifest keratoconus, and individuals with unilateral keratoconus. Special attention will be given to clinically unaffected fellow eyes, which may contain early subclinical changes. This group enables within-subject comparison of a clinically affected eye with a fellow eye that may represent a pre-symptomatic state. To support this analysis, a dedicated image-processing algorithm has been developed, enabling automated identification and analysis of speckle patterns in OCT corneal images. The algorithm is designed to extract and evaluate speckle-related features that may reflect differences in corneal microstructure across the studied groups, with the aim of identifying parameters capable of distinguishing healthy corneas from those exhibiting early keratoconic changes. The findings of this study may contribute to the advancement of non-invasive corneal diagnostics and support the development of automated screening tools applicable in clinical and optometric practice.

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Molecular Dynamics of hSGLT1: How the MAP17 Subunit Guides Transporter Regulation

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Keywords: Membrane Transporter, Molecular Dynamics, Allosteric Regulation, MAP17 (PDZKIP1)

Abstract

Human sodium-glucose cotransporter 1 (hSGLT1) drives critical dietary glucose uptake[1]. While recent cryoEM milestones have resolved static snapshots of the hSGLT1-MAP17 complex[2], a fundamental gap remains in our understanding of how MAP17 physically guides the transporter's conformational transitions. Here, we deployed all-atom molecular dynamics (MD) simulations to capture the real-time, dynamic landscape governing this auxiliary regulation. To achieve this, the systems were embedded in a 3:1 POPC/cholesterol bilayer with 0.15 M NaCl using CHARMM-GUI. Because experimental structures lacked sodium ions, Na⁺ ions were explicitly coordinated into the respective binding sites of both systems. Molecular dynamics simulations were performed using NAMD 3.0.1 with the CHARMM36m force field and TIP3P water model at 303.15 K. Systems were equilibrated for 100 ns prior to a 500 ns production run.

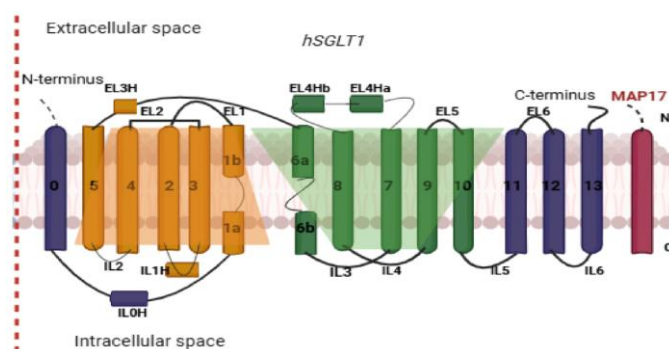


Fig. 1 Topology of the hSGLT1-MAP17 Complex

Comparative trajectories revealed that the uncomplexed hSGLT1 monomer exhibits broad, unconstrained conformational drift across a high-entropy landscape with a negligible free energy barrier (<1.0 kcal/mol). Conversely, MAP17 complexation reconfigures this surface into a directed allosteric funnel. This structural stabilization is anchored by a persistent hydrophobic/aromatic "zipper" at the TM13-MAP17 interface, dominated by TYR662-PRO29 (100% occupancy) and reinforced by VAL653-PHE40 (99.9%) and PHE658-GLY33 (99.7%). This interfacial rigidification initiates a concerted allosteric cascade within a 290–340 ns simulation time. Triggered by spontaneous Na₃ ion dissociation, this event decouples the sodium coordination site and drives a synchronized structural compaction across the transporter. These rearrangements define a spontaneous transition from an outward-open state to a stable, pre-occluded, transport-competent intermediate. This establishes a quantitative framework for how single-transmembrane subunits eliminate conformational degeneracy to direct transporter trajectories, offering novel insights for selective therapeutic design.

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Lipid-Tail Dynamics of AM404 Revealed by ATR-FTIR and DFT-informed Molecular Dynamics

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Keywords: AM404, paracetamol metabolite, Molecular Dynamics, DFT, FTIR

Abstract

Acetaminophen, commonly known as paracetamol, was introduced to the market in 1955 and remains one of the widely used over-the-counter (OTC) drugs in the world [1]. It is present in numerous medications and is renowned for its safety profile and effectiveness in treating mild-to-moderate pain [2]. Despite its widespread use, its mechanism of action remains not fully understood. Recent studies suggest that the pharmacological activity of acetaminophen may be mediated not only by the parent molecule itself, but also by its metabolites [3]. One of them is AM404, a bioactive metabolite of acetaminophen (paracetamol) [4]. It is considered an important contributor to the drug's analgesic and antipyretic effects [5]. However, its molecular structure and temperature-dependent conformational behavior have not yet been characterized in detail. In this work, the conformational dynamics of AM404 in the 37–45 °C range were studied using ATR-FTIR spectroscopy combined with molecular dynamics simulations and DFT calculations. Experimental spectra were compared with spectra calculated for MD-derived conformers to identify temperature-sensitive vibrational features and relate them to changes in molecular geometry. The results show that AM404 retains a dominant conformational state across the investigated temperature range, while temperature changes alter the distribution of trans and gauche rotameric states. These changes are localized mainly in the lipid chain, whereas the aromatic-amide region remains structurally stable. The combined spectroscopic and computational approach provides reference data for the identification of AM404 and offers insight into its conformational flexibility under physiologically relevant conditions.

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POSTER PRESENTATIONS

Discrepancies in the chemical composition of commercially available resin-based dental pit and fissure sealants

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Keywords: Resin-based dental sealants, Dental materials safety, Market transparency, CAS registry, Filler content, Safety datasheets

Abstract

Dental sealants are widely used in dentistry, but their exact chemical composition is often hard to trace. In this study, the discrepancies and gaps in commercial pit and fissure sealants formulations were investigated. A review of 52 chemical formulations from 41 different products was carried out by comparing official Safety Data Sheets (SDS) with scientific literature [1].

The results indicated a lack of market transparency. Out of 116 unique ingredients found in the products, only 41 had a Chemical Abstracts Service number assigned. Reporting of 75 remaining ingredients did not allow for proper CAS assignment (Fig.1). In some formulations, independent studies found monomers and fluoride sources that were undisclosed in the official manufacturer documentation (depending on regional regulations). The absence of clear reporting makes it challenging to assess safety and long-term behavior for patients. To conclude, the findings underlines that the dental industry needs to adapt more reliable reporting regulations in order to help dental practitioners make suitable choices to benefit their patients oral health.

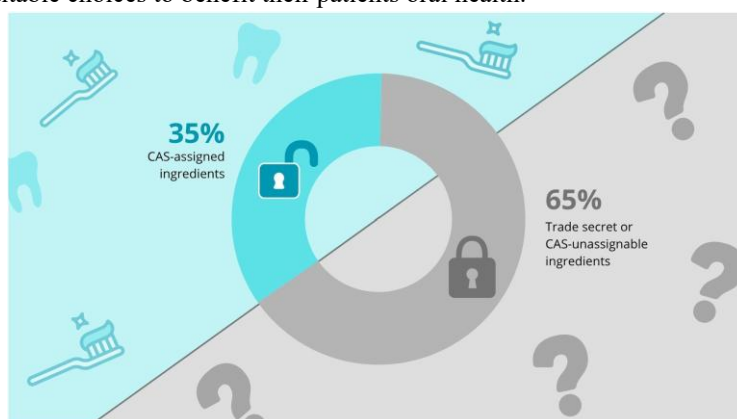


Fig. 1 Composition disclosure gap in commercial resin-based dental sealants.

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Surface Wettability as a Design Parameter for Antimicrobial Nanocomposite Coatings

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Keywords: Antimicrobial coatings, Surface wettability, Carbon nanotubes, Halloysite nanotubes

Abstract

Antimicrobial resistance (AMR) is a growing global threat, responsible for 1.2 million deaths in 2021 and linked to nearly 5 million more. These numbers are projected to rise significantly by 2050 [1]. With the slow pace and high cost of new drug development, alternative strategies are urgently needed. Antimicrobial coatings offer a promising solution by preventing biofilm formation, a key factor in AMR due to its extreme resilience. These coatings work through antifouling (preventing microbial adhesion) and antimicrobial (killing or inhibiting microbes) mechanisms.

Surface wettability is a critical factor governing the mode of action of antimicrobial coatings. Hydrophobicity can hinder microbial adhesion and disrupt cellular structures like bacterial fimbriae. This property can be achieved using nanoparticles, such as multiwalled carbon nanotubes (MWCNTs), which increase surface roughness to create hierarchical structures. In contrast, hydrophilic coatings can provide antimicrobial benefits in functionalized systems that require water-mediated activity, such as antimicrobial photodynamic inactivation (aPDI), where reactive oxygen species (ROS) generation depends on local hydration [2]. In this context, halloysite nanotubes (HNTs) are promising candidates for such applications due to their tubular morphology, biocompatibility, and capacity to act as carriers for active compounds.

In this study, coatings containing MWCNTs or HNTs suspended in a silica sol-gel matrix were fabricated and characterized. Contact angle measurements and OCT-based roughness analysis demonstrated that nanotube incorporation significantly altered surface properties. MWCNT-containing coatings exhibited increased hydrophobicity, particularly in sonicated and double-layer variants, which correlated with enhanced surface roughness. In contrast, HNT-based coatings remained hydrophilic, highlighting their suitability for applications where surface hydration is advantageous.

The results demonstrate that nanostructure-driven wettability tuning provides a versatile strategy for designing surfaces with application-specific antimicrobial mechanisms, ranging from antifouling hydrophobic barriers to hydrophilic, ROS-supporting functional coatings.

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Peptide Nucleic Acid Monomers: A Quantum Chemical Study with Implications for PNA-Based Biomedical Applications

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Keywords: peptide nucleic acid, gene therapy, biosensor, hydrolytic stability, computational chemistry

Abstract

Peptide nucleic acids (PNAs) have emerged as one of the most promising synthetic biomolecules in modern biomedical engineering [1], with established and emerging applications in antisense gene silencing, antigene therapy, sequence specific molecular diagnostics, and nucleic acid biosensor development [2]. Unlike natural DNA and RNA, PNA carries an electrically neutral peptide-like backbone that renders it invisible to nucleases and proteases, allowing it to survive in biological fluids far longer than its natural counterparts. This biostability is central to the therapeutic and diagnostic utility of PNA, yet the precise chemical mechanism underlying this resistance to hydrolytic degradation has never been quantitatively established at the molecular level. Understanding this mechanism is not merely of academic interest. it is a prerequisite for the rational engineering of PNA sequences with optimised stability profiles suited to specific biomedical environments, from intracellular gene silencing to implantable biosensor platforms. In this work, we address this gap through a high-level quantum chemical investigation of the spontaneous, uncatalysed hydrolysis of all four PNA nucleoside monomers adenine (mA), cytosine (mC), thymine (mT), and guanine (mG) in aqueous solution.

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Investigation of similarity and causality between intracranial and arterial blood pressure signals in neurocritical care patients

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Keywords: traumatic brain injury, intracranial pressure, arterial blood pressure, Granger causality, transfer entropy

Abstract

Background: Intracranial pressure (ICP) and arterial blood pressure (ABP) are the most crucial parameters monitored in traumatic brain injury (TBI) patients [1]. Previous studies have focused mainly on the relationships between ICP and ABP in the slow wave frequency range (below 0.05 Hz), which reflect longer-term vasogenic and autoregulatory mechanisms [2]. The pulse waveform (PW, frequency range ~1 Hz) is related to changes in blood volume over a single cardiac cycle and believed to reflect the cerebrospinal pressure–volume balance [3]. However, despite physiological links, the relationships between ICP and ABP PWs have not been quantitatively investigated before.

Materials and Methods: This study was conducted as a retrospective analysis of data collected in the CENTER-TBI project, with approval from the CENTER-TBI committee (No. 612). The analysis was carried out on a subgroup of 186 adult patients diagnosed with severe TBI. ICP was measured using intra-parenchymal strain gauge or parenchymal fiber optic pressure. ABP was measured using arterial lines. The signals' amplitudes (AmpICP and AmpABP, respectively) were calculated in subsequent, non-overlapping 10-s windows over the first 24 hours of each recording and used as the PW metrics for the analysis. Spearman correlation was computed as a measure of the similarity in time courses of AmpICP and AmpABP. Granger causality (GC) and transfer entropy (TE) were computed in the direction from AmpABP to AmpICP for lags 1 through 6 (10–60 s). The Mann–Whitney test was applied to determine whether there are significant differences between outcome groups (dead vs alive at discharge) and age groups (51 y.o. or younger vs older than 51 y.o.). Statistical analysis for TE was not performed due to few significant values.

Results: Most of the patients exhibited significant correlation coefficients between AmpABP and AmpICP (0.10 [0.03–0.21]). There was a statistically significant difference between alive and deceased patients ($p < 0.001$, 0.09 [0.02–0.18] vs 0.21 [0.16–0.44]), but no statistically significant difference between younger and older patients. The causality analysis showed most GC values were significant (between 57% for lag 1 and 82% for lags 5 and 6). There were no significant differences between alive and deceased patients. However, there was a significant difference between younger and older patients, but only for lags 2 through 6.

Conclusions: The results indicate significant correlations and causal relationships between pulse amplitudes of ABP and ICP in TBI patients. Correlation analysis showed differences between outcome groups while a relationship between older age and higher values has been observed only for GC (AmpABP→AmpICP). As the metrics used in this study showed results in only partial agreement, further studies should focus on more granular analyses and the inclusion of additional factors.

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Miniproteins that selectively bind peptides

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Keywords: Miniproteins, *de novo* protein design, α -helical proteins, SPPS, protein stability, circular dichroism spectroscopy, nanoDSF, synthetic proteins

Abstract

Miniproteins are small proteins consisting of 20 to 70 amino acids, typically defined by a molecular weight not exceeding 10 kDa. They possess well-defined three-dimensional structures that ensure high structural stability and functional specificity. Their conformational structure is stabilized by one of three types of interaction: hydrophobic core, disulfide bridges, or metal complexation [1]. These molecules combine unique properties that make them a promising scaffold for medicinal applications. Miniproteins retain the functional versatility characteristic of natural proteins while remaining accessible to efficient solid-phase synthesis. This chemical approach enables precise sequence control and the incorporation of non-canonical functional groups [1,2]. Furthermore, their small size facilitates cell penetration, enhances manufacturing flexibility, and supports efficient computational design [3]. This research focuses on a novel class of *de novo* four-helix miniproteins designed to form a selective peptide-binding cavity. Their well-defined architecture and high modifiability make them attractive platforms for the development of functional systems such as detection tools, drug delivery carriers, or catalysts. The primary goal achieved to date is the synthesis of these structurally stable frameworks to provide a foundation for future structural and functional studies. The experimental strategy involved the design of orthogonal four-helix scaffolds, which were then synthesized using automated flow solid-phase peptide synthesis (flow-SPPS) using Fmoc chemistry. To date, five different models of four-helix miniproteins have been successfully synthesized, with sequences ranging between 62 and 67 amino acids in length. UV monitoring during the synthesis of these models confirmed high coupling efficiency, as indicated by stable peak intensities, despite the cumulative steric effects typical of such long and demanding sequences.

Acknowledgments

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Directed Horizontal Visibility Graph and HRV Analysis of Neurocardiac Coupling During Hypercapnia-Induced Physiological Stress

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Keywords: directed horizontal visibility graphs, heart rate variability, hypercapnia, neurocardiac coupling, cerebral hemodynamics

Abstract

Introduction to the field: Cardio- and cerebrovascular dynamics are inherently nonlinear and non-stationary, particularly under physiological stress where signals exhibit high variability. Traditional time-frequency methods often prove difficult to interpret in these contexts. The Directed Horizontal Visibility Graph (dHVG) is an advanced method that transforms time series into a network, preserving complex topological properties and providing a robust framework for analyzing signal organization [1] alongside traditional Heart Rate Variability (HRV) metrics.

Background and rationale: Hypercapnia serves as a model for cerebral blood flow impairment by altering cerebrovascular and autonomic regulation [2]. This study evaluates neurocardiac consistency during normocapnia and hypercapnia using dHVG applied to Pulsatility Index (PI) and R–R interval (RR) series and HRV metrics. We employed the Adjusted Rand Index (ARI) to quantify grouping similarity between the two systems and Canonical Correlation Analysis (CCA) to determine the maximum strength of their global coupling.

Main findings and conclusions: Our analysis showed that hypercapnia disrupts predictable physiological patterns. In the heart (RR), the most important changes were found in complexity measures like HRV-PIP (Percentage of inflection points) and HRV-CSI (Cardiac Sympathetic Index). In the brain (PI), graph metrics like local clustering coefficient and graph energy dominated. Interestingly, while the heart and brain remained strongly connected (high canonical correlation > 0.88), they no longer fell into neat, similar groups (low ARI = -0.0302). This suggests that while the two systems are still communicating, the "simulated disorder" causes subjects to react in highly personalized ways.

Broader context: These findings indicate that hypercapnia-induced stress does not break the link between the heart and the brain. Instead, it shifts their interaction into a wide, continuous spectrum. In a healthy state, people react similarly; however, under the stress of hypercapnia, individual differences become dominant. Each person develops a unique physiological "signature" of stress. dHVG and non-linear HRV features are sensitive enough to capture these personalized shifts, providing a powerful tool for monitoring how different individuals cope with physiological disorders.

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Preliminary Research on Wearable Heart Rate Monitoring and Telemetry Limitations in National-Level Swimming Training

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Keywords: wearable sensors, heart rate monitoring, telemetry, internal load, competitive swimming

Abstract

Wearable devices for biosignals monitoring can support high-performance sport practices. They may provide objective, real-time feedback, which clarifies the athlete's physiological response to the exercise [1]. In swimming, this is highly significant since external load, represented by pace, distance and split times, may differ from internal load, reflected by cardiovascular response [2]. The aim of this single-athlete case study was to demonstrate the use of wearable heart rate (HR) sensors for within-session load adjustment during preparation for a national-level swimming competition, with particular focus on technical limitations of live telemetry in pool conditions.

A Polar Verity Sense optical sensor mounted near the temple on swimming goggles was used to collect heart rate data, which were recorded locally for post-session analysis and transmitted live to an Apple iPad Air (M2) used by the coach. The tablet was placed 8 m from the pool wall on the recovery side, and the athlete's maximal HR (201 bpm) was used to define five heart rate zones.

Three representative training sessions were analyzed: recovery/aerobic, threshold-oriented and high-intensity anaerobic. HR response was compared with split times, rest intervals, intended training intensity and real-time data availability. Additionally, 10 training records were evaluated in order to examine the influence of the Bluetooth connection quality on the transmitted HR values.

Real-time HR feedback was most valuable during breaks and between repetitions, where it supported pace correction and rest-interval adjustment. In the threshold-oriented session, HR frequently reached the same value of 181 bpm during a 5 x 200 m set in opposite to the fact that split times were progressively slowing down. It was reliable sign of increase in internal load, moreover those results helped with adjustment of rest extension and pace. In the high-intensity anaerobic session, HR increased across repeated 50 m efforts, while the final maximal repetition showed a clear performance drop, suggesting accumulated metabolic fatigue [3]. In the recovery/aerobic session, HR feedback helped maintain the intended low-to-moderate intensity in aerobic endurance zone.

Live-time telemetry represented the main technical limitation. Since Bluetooth transmission at 2.4 GHz is strongly attenuated by water, repeated sensor submersion reduced real-time data availability in pool conditions [4]. Across 10 analyzed sessions, connection quality ranged from 81% to 90%. Data recorded directly by the sensor were compared with values displayed on the tablet. The mean relative error across all HR zones was 3min 1s (28.9%). The largest relative error occurred in HR zone 1 (7min 12s; 42.5%) due to transmission losses being classified into this zone, while the highest percentage error was observed in the shortest, high-intensity HR zone 5 (21s; 74.8%). For HR zones 2–4, percentage errors ranged from 9.8% to 13.6%. Mean relative error decreased with higher connection quality from 4min 2s to 1min 41s. Additionally, tablet-based feedback showed a delay of ~2–5s. These findings indicate that Bluetooth transmission quality substantially affects HR classification accuracy, particularly during short high-intensity efforts, limiting the reliability of real-time feedback in competitive swimming.

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Numerical Analysis of the Functional Behavior of a Full Dental Arch under Various Attachment Strategies to Patient Tissues

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

Abstract

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-ptyergoid implants in the distal region. They were analyzed under defined boundary conditions and three loading scenarios: biting on the distal tooth, unilateral mastication, and central occlusion. Stress, strain and displacement distributions were evaluated to compare the biomechanical stability and safety of both configurations.



Fig. 1 Geometric model of the M6 maxillary full-arch prosthesis with distal tubero-ptyergoid implant support.

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-ptyergoid 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.

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Membrane Scaffolding and Lipid Rigidification Induced by Crotonamine from *Crotalus durissus terrificus*: A Molecular Dynamics Study

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Keywords: molecular dynamics simulation, crotonamine, erythrocyte membrane, cell-penetrating peptides, lipid bilayer

Abstract

Background: Snake venom peptides with cell-penetrating properties are of growing interest in biomedical engineering due to their potential as drug delivery vehicles. Crotonamine, a 42-amino-acid polypeptide from the venom of the South American rattlesnake (*Crotalus durissus terrificus*), is known to cross lipid bilayers without destroying them, despite carrying a strong net positive charge. The molecular mechanism underlying this interaction, particularly its effect on membrane structural properties, remains poorly understood.

Aim: The aim of this study was to characterize the structural dynamics of Crotonamine and an erythrocyte membrane model during early-stage binding using Molecular Dynamics (MD) simulations.

Materials and Methods: Full-atom MD simulations were performed using NAMD 2.14 with the CHARMM36 force field. An asymmetric lipid bilayer was constructed to reflect the physiological composition of the red blood cell plasma membrane (outer leaflet: 40% Cholesterol, 30% PSM, 30% POPC; inner leaflet: 30% Cholesterol, 40% POPE, 20% POPS, 10% POPC). A peptide-free control membrane was simulated for 20 ns as a baseline. The Crotonamine structure (PDB ID: 1H5O) was equilibrated in solvent for 32 ns, then placed at the outer leaflet surface, and the peptide-membrane complex was simulated for 20 ns in the NPT ensemble at physiological conditions (310.7 K, 0.15 M NaCl). Peptide structural stability was assessed by backbone RMSD and end-to-end distance; membrane properties were quantified by area per lipid (APL), bilayer thickness, deuterium order parameters (S_{CD}), lipid tilt angle distributions, and lateral diffusion coefficients.

Results: The erythrocyte membrane surface acted as a stabilizing scaffold for Crotonamine. While the peptide exhibited high conformational flexibility in bulk solvent ($RMSD = 8.1 \pm 1.0 \text{ \AA}$), binding to the lipid interface induced a rapid folding event at approximately 4 ns, stabilizing the peptide into a compact conformation ($RMSD = 4.1 \pm 0.3 \text{ \AA}$) with the end-to-end distance dropping from $21.9 \pm 4.8 \text{ \AA}$ to $6.5 \pm 2.5 \text{ \AA}$. Ramachandran analysis confirmed that the membrane-bound structure retained stereochemical validity without denaturation. Regarding membrane mechanics, the interaction caused a localized increase in lipid tail order parameters restricted to the upper acyl chain region (C3-C8), attributed to electrostatic locking between the basic residues of the peptide (Lys, Arg) and the phospholipid headgroups. This surface rigidification, comparable in character to effects reported for inhalation anesthetics, was supported by a shift in mean lipid tilt angle from 15.8° to 12.4° , contributing to a slight bilayer thickening. The deep hydrophobic core (C9-C12) remained unaffected, confirming the absence of a global phase transition.

Conclusion: MD simulations revealed that Crotonamine interacts with the erythrocyte membrane through a two-sided mechanism: the lipid surface locks the peptide into a folded, functional conformation, while the peptide in turn rigidifies the headgroup region via electrostatic anchoring without disrupting overall membrane fluidity. These findings contribute to the mechanistic understanding of how cell-penetrating peptides interact with biological membranes and suggest that molecular dynamics simulations can serve as a valuable tool for characterizing such interactions at the atomic level.

2,6-Diaminopurine: a Non-Canonical Nucleobase With Potential Roles in Prebiotic Chemistry

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Keywords: 2,6-diaminopurine, nonenzymatic RNA replication, prebiotic chemistry, molecular dynamics

Abstract

2,6-Diaminopurine (D) is a non-canonical purine nucleobase that differs from adenine by an additional amino group at the C2 position. Though non-canonical, it occurs in nature, notably in the genome of cyanophage S-2L, where it replaces adenine entirely. [1]. This substitution is enabled by D forming three hydrogen bonds with uracil, compared to two in standard A:U pairs, resulting in significantly more stable nucleic acid duplexes.

This enhanced base pairing has consequences at multiple levels. In nonenzymatic RNA replication, a process considered essential for the transmission of genetic information before the emergence of enzymatic machinery, D-containing activated dinucleotides bind their uracil template with substantially higher affinity than adenine counterparts, improving both yield and fidelity of primer extension [2, 3]

Molecular dynamics simulations were performed to investigate the structural basis of D's role in nonenzymatic replication. D-containing activated dinucleotides bound to a uracil RNA template were found to maintain stable Watson-Crick base pairing and to frequently sample conformations with favorable geometry for primer extension. These findings provide molecular-level insight into the potential role of 2,6-diaminopurine in the early chemical evolution of nucleic acids.

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In Silico Design and Functional Optimization of Antimicrobial Peptides Targeting Drug Resistant Fungal Infections

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Keywords: AI, Antimicrobial peptides, Drug Resistance, Fungal infections, Immune Response

Abstract

Infectious diseases driven by drug-resistant fungal pathogens represent a rapidly growing global health crisis, particularly for vulnerable hospital patients with weakened immune systems. Right now, medicine is running out of options because these aggressive fungi have learned to evade our few existing antifungal drugs [1]. While nature produces defensive molecules called antimicrobial peptides (AMPs) that can destroy these pathogens, fungi have evolved a brutal counter defense: they secrete specialized defense that quickly chops up and neutralize our treatments before they can work [2, 3]. This research addresses this urgent medical bottleneck by combining artificial intelligence and computational biology to design a new class of synthetic treatments. Instead of using traditional, slow laboratory trial-and-error, this project establishes an automated, high-speed AI pipeline to design a functional molecule. These advanced molecules work as they bypass external defenses, acting as a magnetic homing beacon that guides the patient's own human immune cells to actively hunt down and devour the infection. To ensure these treatments survive the harsh environment of an infection, the project uses a data-driven computer funnel. First, a generative AI network screens thousands of natural defense sequences to write non-toxic molecule blueprints. Next, advanced structural software simulates exactly how these new shapes fit into human immune receptors. Ultimately, the top computer-optimized AMP candidates will be synthesized and tested in a cell-free lab environment. By incubating them with real proteases and tracking their survival, the research will provide a highly stable, low-cost therapeutic AMPs. This project will deliver a fast, open-source drug discovery platform to help the pharmaceutical industry develop life-saving treatments against currently untreatable superbug infections.

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Optimizing Exercise Performance Through Cognitive Functions

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Keywords: biomechanics, attention of focus, optimization, motor learning, cognitive functions

Abstract

Background: Optimizing exercise performance is important not only for competitive athletes, but also in clinical rehabilitation settings. One underexplored aspect of rehabilitation is the role of attentional focus strategies in shaping biomechanical outcomes during exercises commonly used in recovery protocols, such as the split squat jump commonly used in rehabilitation after anterior cruciate ligament reconstruction.

Aim: The aim of this study was to compare the effects of external and internal focus of attention on biomechanical outcomes of the split squat jump exercise used in rehabilitation.

Materials and Methods: Twenty-seven healthy young adults (18 females, 9 males) participated in this study. Three-dimensional positions of the lower back and bilateral lateral ankles were tracked using the OptiTrack motion capture system. Each participant performed two sets of eight split squat jumps, once under internal focus inducing instruction, which focused their attention on their body, and once under external focus inducing instruction, which focused their attention on the goal of the exercise. Time of flight and height of flight were calculated using the back marker, and split distance was calculated using the lateral ankle markers. The influence of focus type on exercise performance was assessed using a non-parametric test, as the data did not follow a normal distribution.

Results: Figure 1 presents boxplots of three parameters comparing external and internal focus of attention conditions. Statistical analysis showed that two out of three parameters were significantly affected by the focus condition. Height of flight was significantly higher under the external focus condition ($p = 0.04$), while time of flight was significantly longer under the internal focus condition ($p = 0.001$). No significant difference was observed for split distance ($p = 0.07$).

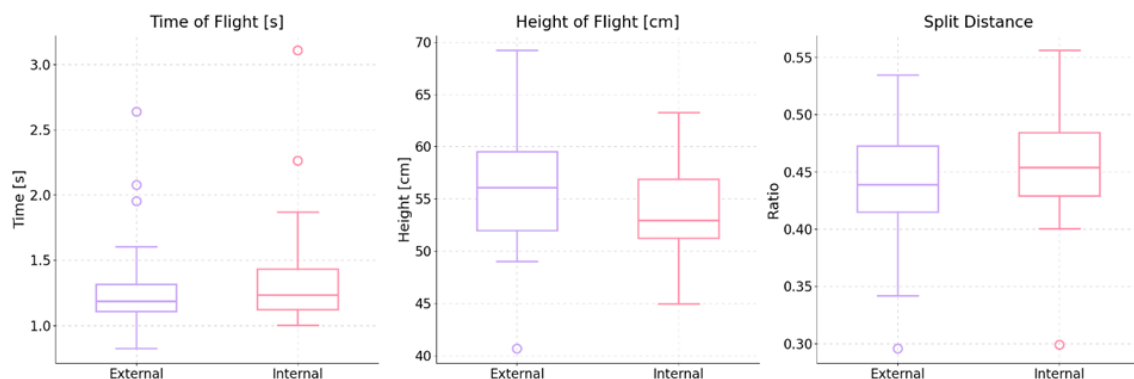


Fig. 1 Boxplots comparing time of flight, height of flight, and split distance between external and internal focus of attention conditions.

Conclusion: The focus of attention significantly influenced two out of three biomechanical parameters of the split squat jump. External focus of attention resulted in higher jumps, while internal focus produced longer flight times. These findings suggest that the choice of attentional focus instruction given by physiotherapists during rehabilitation exercises can meaningfully affect patient performance outcomes.

Egocentric Resilience, Allocentric Decline: A VR-Based Dissociation of Spatial Memory Across the Lifespan

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Keywords: spatial memory, aging, virtual reality, allocentric navigation, hippocampal decline

Abstract

Background: Where you are and where things are relative to each other — these two senses of space are processed by distinct neural systems, and they do not age equally. While egocentric memory remains relatively preserved in older adults, allocentric memory — the hippocampal ability to build cognitive maps — deteriorates disproportionately. Capturing this dissociation has remained methodologically elusive due to confounding factors in real-world tasks.

Aim: The aim of this study was to isolate both spatial reference frames within a single session using a minimalist VR protocol to identify specific signatures of spatial decline.

Materials and Methods: Fifty participants (30 young adults, 18–35; 20 older adults, 55+) completed 32 egocentric and 32 allocentric ball-placement trials using Meta Quest 3. The allocentric subtest introduced scene rotation during recall to force genuine coordinate transformation.

Results: Older adults performed 34% worse on egocentric trials and 91% worse on allocentric trials. The Egocentric-to-Allocentric Ratio (EAR) was significantly lower in older adults (0.57 vs. 0.79, $p = 0.001$). Egocentric error scaled with target distance from center (signal-dependent noise), while allocentric error scaled with the target's distance from the nearest reference landmark, reflecting distinct mechanistic error signatures.

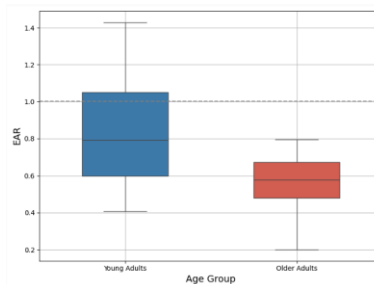


Fig. 1 Distribution of Egocentric-to-Allocentric Ratio (EAR) for young (blue) and older adults (red). EAR is the ratio of median egocentric to allocentric placement errors. Boxplots show group distributions with medians indicated; outliers are excluded.

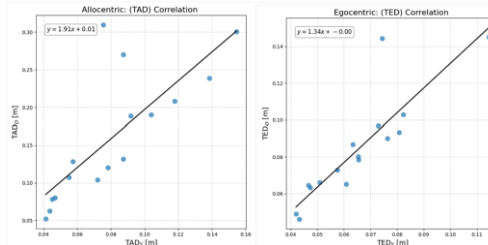


Fig. 2 (a) Egocentric Error (TED): Median group errors across 16 trial settings for older (TEDo) vs. young adults (TEDy). Solid line indicates linear regression ($\beta = 1.34$, Spearman's $\rho = 0.94$, $p < 0.001$). (b) Allocentric Error (TAD): Median group errors across 16 trial settings for older (TADo) vs. young adults (TADy). Solid line indicates linear regression ($\beta = 1.91$, Spearman's $\rho = 0.83$, $p < 0.001$)

Conclusion: These results establish the EAR as a sensitive, interpretable biomarker for hippocampal-linked spatial decline, offering significant potential for clinical screening. While age-related degradation was evident across both reference frames, the disproportionate allocentric deficit underscores spatial memory impairment as a hallmark of the aging brain.

Hybrid Fermentation Modeling with Sensor-Conditioned Multi-Structure Kinetics

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Keywords: Hybrid modeling; bioprocess; fermentation; *Saccharomyces cerevisiae*; multi-structure kinetics;

Abstract

Mechanistic fermentation models encode mass-balance equations and pre-specified kinetic laws, but are typically limited to a single, fixed kinetic expression - reducing their ability to represent variable batch conditions. A purely data-driven approach, on the other hand, ignores what is already known about fermentation biology [1].

We propose a hybrid fermentation model for *S. cerevisiae* (baker's yeast, a widely used industrial microorganism) that combines structured mass-balance state equations with a data-weighted combination of three kinetic formulations: Monod (substrate-limited growth), Contois (biomass-density-dependent growth), and Haldane (substrate-inhibited growth) [2–4]. Rather than pre-selecting one kinetic expression, the model infers the dominant kinetic regime from online process sensor signals (pH, dissolved oxygen, temperature) via a trainable weighting function, preserving physical interpretability while enabling adaptation to batch-specific dynamics.

The approach was evaluated on a synthetic *S. cerevisiae* fermentation dataset of 50 batches (train: 1–45, validation: 46–50). Biomass (X, cell mass concentration), glucose (S, carbon source), and ethanol (E, overflow metabolite) were predicted simultaneously; the best model was selected by minimising a weighted composite of prediction error (RMSE) across all three outputs. All predictions satisfied non-negativity and predefined physiological range constraints.

The hybrid model achieved RMSE of 1.23 g/L (X), 0.59 g/L (S), and 0.47 g/L (E). Against a Monod-only reference trained under identical conditions, prediction error was reduced by 11% (X), 21% (S), and 39% (E). The dominant inferred kinetic structure was Monod-type (~91%); predicted ethanol peaks matched observed peak times exactly across all validation batches (timing error: 0 h).

Multi-structure hybrid kinetics outperformed the single-structure reference across all outputs, with the largest gain in ethanol - the variable most sensitive to the Crabtree overflow metabolism of *S. cerevisiae* [5]. These results demonstrate that adaptive kinetic weighing can be an effective strategy to improve the accuracy of fermentation models. Prospective validation under real bioreactor conditions is ongoing.

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From Population Analysis to the Single-Cell Level: Development of Flow Cytometric Procedures for Studying *In Vitro* Erythrocyte Aging

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Keywords: red blood cells, storage lesion, osmotic fragility, flow cytometry

Abstract

Previous studies on the aging of erythrocytes stored in SAGM preservation medium have allowed for the characterization of their population properties, including changes in osmotic fragility, morphological parameters assessed with the Mindray BC-2800 hemoanalyzer. While these methods provide valuable data regarding the overall state of the sample, they do not allow for the precise monitoring of the heterogeneity of changes occurring at the level of individual cells.

To enable a complementary analysis of aging dynamics, it became necessary to develop and optimize dedicated flow cytometric procedures. Within the framework of preliminary research, measurement protocols were established to monitor the condition of erythrocytes within populations. A key element was the utilization of light scattering parameters—Forward Scatter (FSC) and Side Scatter (SSC)—to create characteristic dot plots, which allow for the morphological differentiation of "young" and "old" sub-populations based on changes in volume and granularity. To deepen the functional analysis, fluorescent staining procedures were implemented using Calcein AM to assess membrane integrity and metabolic viability, Fluo-4 AM to monitor intracellular calcium (Ca^{2+}) concentrations, and Annexin V for the detection of early-stage eryptosis via phosphatidylserine exposure. These developed methodologies allow for a transition from a general assessment of hemolysis and morphology to the precise physiological mapping of individual red blood cells (Fig.1).

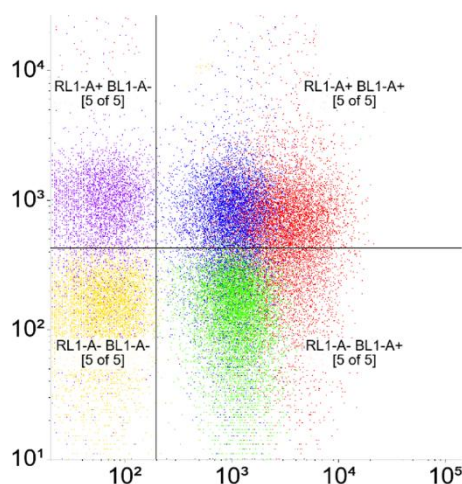


Fig. 1 Representative flow cytometry dot plot of erythrocyte analysis. X-axis: Calcein AM fluorescence (viability marker); Y-axis: Annexin V-APC fluorescence (eryptosis marker).

Such an integrated research approach provides a robust foundation for further analysis of the mechanisms of erythrocyte degradation during *in vitro* storage and may contribute to a better understanding of the phenomenon of storage lesions.

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Computer-aided design and finite element analysis of personalized orthotic insoles for flatfoot correction

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Keywords: Orthotic insoles, flatfoot, foot diagnostics, thermoplastic polyurethane (TPU), finite element method (FEM)

Abstract

Personalized foot orthoses are increasingly developed using computer-aided workflows and additive manufacturing, which enable patient-specific geometry and material-property tailoring [1,2]. This study aimed to develop a measurement-based workflow for the design and numerical assessment of personalized orthotic insoles intended for flatfoot correction.

Foot diagnostics were performed using a CQStopy3D podoscope, CQ-KAM image analysis of hindfoot alignment, and FreeMED MAXI pedobarographic measurements under static and dynamic conditions. Based on these data, separate CAD models of the left and right insoles were prepared. Two thermoplastic polyurethane materials with Shore D hardnesses of 20D and 40D were characterized in uniaxial compression using an MTS 858 Mini Bionix testing machine to determine apparent tangent elastic moduli for numerical modelling. Finite element analysis was carried out in Ansys Workbench 2024 R1 to evaluate equivalent von Mises stresses and equivalent strains under forefoot and hindfoot loads derived from the static plantar-force distribution. The overall experimental and computational workflow is summarized in Fig. 1.

The apparent tangent elastic moduli were 18.5 ± 0.4 MPa for TPU 20D and 30.6 ± 3.3 MPa for TPU 40D. The maximum equivalent stresses were 0.189 MPa for the left insole and 0.075 MPa for the right insole, with stress concentrations observed mainly in the heel-support region. Increasing TPU hardness reduced maximum equivalent strain from 0.010 to 0.006 mm/mm for the left insole and from 0.005 to 0.003 mm/mm for the right insole. These results indicate that insole geometry and load distribution affected the maximum stress and strain values, whereas material stiffness predominantly governed the deformation response, with no evident effect on maximum stress values in the analysed models. The proposed workflow enables preliminary selection of material and geometry prior to prototyping, although experimental validation under real use conditions is required.

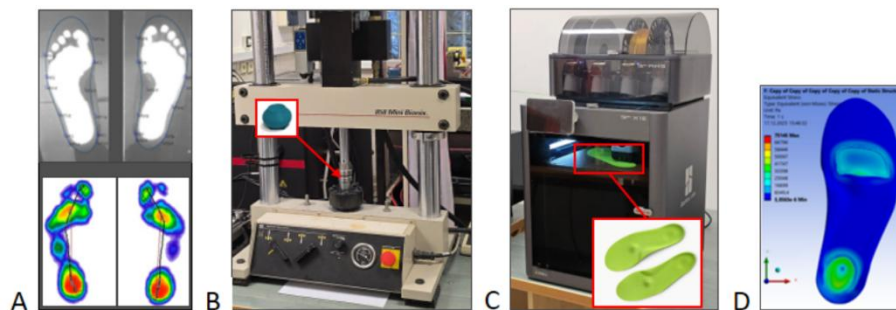


Fig. 1. Study workflow: (A) foot diagnostics; (B) uniaxial compression testing of TPU specimens; (C) representative 3D-printed insoles; (D) finite element analysis of the personalized insole model

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Concept of the Bio Electronic Extremity (BEE) Project

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Keywords: Upper limb prosthesis, Surface electromyography (sEMG), Mechanomyography (MMG), FDM, nylon filaments

Abstract

Nowadays, a popular source of control signal for upper limb prostheses is the electromyographic signal obtained non-invasively, known as sEMG (surface Electromyography) [1]. However, the application of this technique involves a significant challenge, namely the lack of signal universality [2]. This results in the need for thorough customization tailored to the individual parameters as well as the needs of the patient. An additional obstacle is the rigid prosthetic socket, which cannot adapt to changes in the user's anthropometry, when necessary, thereby generating potential maintenance costs.

Due to these emerging issues, the aim of this project is to develop an upper limb prosthesis that eliminates the aforementioned problematic aspects and provides a universal solution. The Bio Electronic Extremity (BEE) prosthesis will aim to analyze the action potential of muscle fibers using electromyography combined with mechanomyography [3], which involves recording surface muscle vibrations. In order to reduce costs, another proposal in the project is to replace the traditional, rigid prosthetic socket with an adjustable structure, where the use of micrometric buckles is considered as one of the potential solutions. On the other hand, regarding the remaining load-bearing structure of the prosthesis, FDM 3D printing is assumed as a potential solution, considering various grades of nylon.

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Structural Changes and Aggregation Kinetics of *Staphylococcus Aureus* PSM α 1 and δ -Toxin

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

Abstract

PSM α 1 and δ -Toxin belong to PSM (Phenol Soluble Modulins) peptide family. They are short functional peptides secreted by the bacteria *Staphylococcus aureus*. They play an essential role in the bacterial life cycle, contributing to bacterial biofilm formation and serving as both structural elements and dispersion agents, as well as enhancing *S. aureus* virulence and defense [1,3]. The aim of the experiment was to verify aggregation propensity and secondary structural distribution of synthetic deformylated variants of PSM α 1 and δ -toxin and comparing results to already existing literature [1,2,3].

The secondary structure composition of PSM α 1 and δ -toxin was studied using ATR-FTIR (Attenuated Total Reflectance Fourier Transform Infrared) and CD (Circular Dichroism) spectroscopy. Both types of spectra were registered for in-water solution of the peptides. The deconvolution of the ATR-FTIR spectra was carried out using a Lorentzian function to identify bands representing secondary structures, such as β -sheets, α -helices, β -turns, and unordered coil. Estimation of secondary structure contributions based on CD spectra were done with BeStSel [4] tool for single spectrum analysis. The aggregation behaviour of studied peptides was estimated using the thioflavin T (ThT) fluorescence assay. For this analysis each sample was incubated in five different concentrations at 37°C for 48 h, fluorescence was measured each 30 minutes to plot kinetics curves of aggregation.

Secondary structure analysis of δ -toxin confirmed that its main components were α -helices and unordered coil. While ATR-FTIR suggested a near-total absence of β -sheets, CD analysis identified a minor fraction of parallel β -sheets, alongside a moderate contribution of β -turns. Both methods consistently showed that PSM α 1 consisted mainly of β -sheets supplemented with a high content of β -turns and disordered regions. PSM α 1 exhibited amyloid fibrillation with logarithmic kinetics, with rapid elongation at the highest studied concentration. In contrast, δ -toxin lacked a logarithmic growth profile and showed no immediate ThT fluorescence increases, at studied concentration range and under used experimental conditions.

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