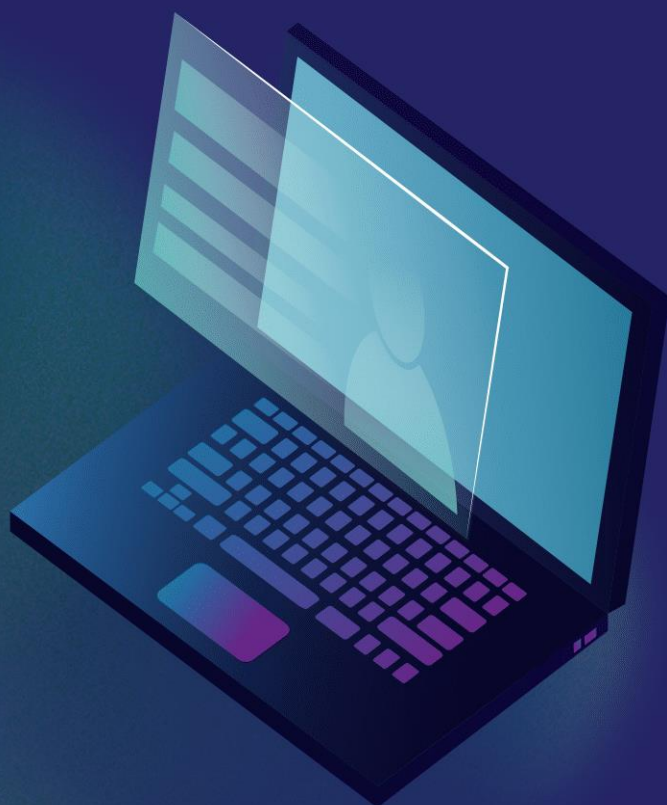


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VIRTUAL BOOK OF
ABSTRACTS

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PhD students
(oral presentations)

Asymmetry Effects in VR Implementation of the Rod and Frame Test

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Background: In the classic Rod-and-Frame Test (RFT), participants align a pivoted rod with the vertical while viewing a slanted, coaxially mounted frame. Traditionally, the frame is thought to cause a direct effect, whereby the rod is rotated past vertical in the direction of the frame's tilt [1]. A fundamental question is whether differences in RFT performance reflect only a general susceptibility to this illusion or instead reflect how individuals process visual context. When aligning the rod with the true vertical, participants may use the frame's edges as visual cues [2]. At larger tilt angles, however, rotating the rod opposite to the frame's tilt – toward its diagonal [2], which approximates the vertical – can actually reduce alignment error [3]. We hypothesize that individuals who adopt this indirect strategy can align the rod more accurately.

Materials and Methods: We developed a Virtual Rod-and-Frame Test (VRRFT) using Unity 3D for the Oculus Quest 3 headset. Fourteen healthy young adults (mean age = 21.36 ± 2.47 years) viewed a virtual 3D corridor and used a controller to align a rod with the vertical across 18 frame tilt angles (-40° to $+45^\circ$, 10 trials per angle). A bias function was defined to take a value of 1 when the rod was rotated toward the frame tilt, and -1 otherwise. The scaled range of this function, referred to as adaptability, was used to quantify changes in alignment strategy.

Results: A significant negative correlation was found between adaptability and mean alignment error. This relationship remained robust when analyzing clockwise and counterclockwise tilt conditions separately.

Conclusion: Our findings suggest that individuals with higher adaptability – i.e., those who switch alignment strategies based on frame tilt – exhibit lower orientation errors. Therefore, RFT error is not solely a measure of visual field dependence but also reflects the strategic processing of visual context.

- [1] H. A. Witkin and S. E. Asch. Studies in space orientation. IV. Further experiments on perception of the upright with displaced visual fields. *J. Exp. Psychol.*, 38(6):762, 1948.
- [2] H. C. Beh, P. M. Wenderoth, and A. T. Purcell. The angular function of a rod-and-frame illusion. *Percept. Psychophys.*, 9:353–355, 1971.
- [3] R. Abdul Razzak and J. Bagust. Perceptual lateralization on the Rod-and-Frame Test in young and older adults. *Appl. Neuropsychol. Adult*, 31(4):405–411, 2024.

Acetaminophen Metabolites as Potential Sodium Channels Inhibitors

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Background: Recent findings have shown that it is not the acetaminophen molecule that is responsible for the analgesic effect, but its metabolites[1]. Especially interesting molecule in this context is N-arachidonoylphenolamine (AM404). Matuuf et al. demonstrated that this particular compound affects the activity of two voltage-gated sodium channels – NaV 1.7 and NaV 1.8 [2]. These molecular machines are mainly expressed in the peripheral nervous system (PNS) and are responsible for pain signal pathways [3]. Such a revelation can be crucial to solving the mystery behind the actual mechanism of action of acetaminophen, and possibly provide new possible research targets for the new generation of analgesic drugs.

Materials and Methods: Initial molecular docking calculations conducted with AM404 and experimental 3D structures of NaV 1.7 and NaV 1.8 have shown that this compound binds to the sodium channels. This information encouraged further studies. For now, experimentally obtained structures of the aforementioned sodium channels are incomplete; thus, there is a need to complete them. This study involves computational approaches for protein modelling. Homology modeling with multiple templates was conducted using MODELLER 10.5 software [4]. Due to the similarities in the architecture of sodium, potassium and calcium channels, it was possible to obtain the structure of NaV 1.7 and NaV 1.8 with the use of three templates – 3D structures of respective sodium channels – NaV 1.7 (PDB ID 6J8G), NaV 1.8 (PDB ID 7WE4), sodium channel from *Periplaneta americana* (PDB ID 5X0M) and calcium channel from *Oryctolagus cuniculus* (PDB ID 6JP8).

Results: Obtained results contain two reliable models of NaV 1.7 and NaV 1.8. The accuracy of models in reference to template structure was measured with RMSD after superpositioning backbones of obtained structures to experimentally obtained 3D structures, yielding the values 0.806 for NaV 1.7 and 0.533 for NaV 1.8, which confirms the high quality of obtained models.

Conclusion: Obtaining high-quality models of sodium channels is crucial for other computational steps, such as molecular dynamics with lipid bilayers, more advanced molecular docking, and molecular dynamics with acetaminophen metabolites. This kind of simulation are crucial for gaining better insight into the molecular mechanism of acetaminophen.

- [1] S. W. Saliba, A. R. Marcotegui, E. Fortwängler, J. Ditrich, J. C. Perazzo, E. Muñoz, A. C. P. de Oliveira, and B. L. Fiebich. AM404, paracetamol metabolite, prevents prostaglandin synthesis in activated microglia by inhibiting COX activity. *J. Neuroinflammation*, 14(1):246, 2017.
- [2] Y. Maatuf, Y. Kushnir, M. Ghantous, A. Iskimov, A. Binshtok, and A. Priel. Paracetamol produces analgesia peripherally via AM404-induced direct inhibition of nociceptive sodium channels. *SSRN Electronic Journal*, 2023.
- [3] F. Zhao, W. Jin, L. Ma, J. Y. Zhang, J. L. Wang, J. H. Zhang, and Y. B. Song. Investigation of the selectivity of one type of small-molecule inhibitor for three Nav channel isoforms based on the method of computer simulation. *J. Biomol. Struct. Dyn.*, 37(3):702–713, 2018.
- [4] B. Webb and A. Šali. Comparative protein structure modeling using MODELLER. *Curr. Protoc. Bioinformatics*, 54:5.6.1–5.6.37, 2016.

Morphological Analysis of Total Hemoglobin Concentration Pulse Waveform and its Relationships with Age

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Background: With aging, the cerebrovascular system undergoes significant structural and functional changes that can impair the regulation of cerebral blood flow. Functional near-infrared spectroscopy (fNIRS) is a non-invasive technique that enables real-time monitoring of pulsatile changes in blood oxygenation and volume within the cerebral cortex. This study investigated the changes in the shape of the total hemoglobin concentration (tHb) pulse waveform with aging including sex-related differences.

Materials and Methods: Continuous records of changes in oxygenated and deoxygenated hemoglobin concentration (HbO, HbR) in the frontal lobe area in a resting state were collected from 57 healthy volunteers in different age (range: 19-66, median: 28, IQR: 22-47 [years], males: 26) using continuous wave fNIRS device. tHb was calculated as a sample-to-sample sum of HbO and HbR. The tHb signal was automatically cut into single pulse waveforms. Each pulse waveform was detrended, linearly interpolated in X axis and normalized along the Y axis. A similarity of the tHb pulse to the triangle was measured using five indices presented in Figure 1. Non-parametric tests were applied due to the rejection of the normality hypothesis for most of the analysed indices based on the Shapiro-Wilk test. Correlations between the variables and age were assessed using Spearman rank test (R_s). Interactions between age group (defined as I for individuals younger than 28 years and II otherwise) and sex and their impact on morphological variables was tested using Scheirer-Ray-Hare test.

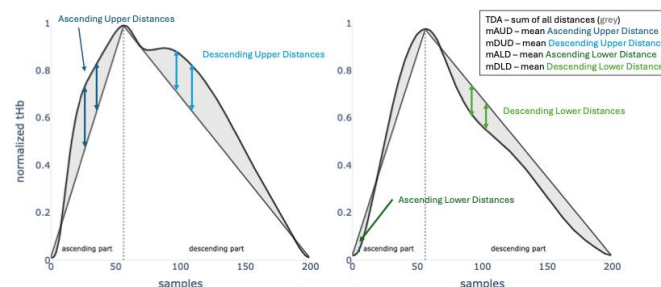


Figure 1. Visualization of a triangle fitted into the total hemoglobin concentration (tHb) pulse waveform and triangle similarity indices in young (25 years) and old (55 years) volunteer.

Results: TDA was negatively correlated with age ($R_s=-0.459$, $p<<0.01$). Among four tested average to-triangle distances, only two metrics were correlated with age: mAUD ($R_s=-0.626$, $p<<0.01$) and mDUD ($R_s=0.283$, $p=0.03$). Sex and age group have significant effect on TDA, mAUD and mDUD, and there is an interaction between these two factors (TDA: $H_{sex}=5.01$, $p_{sex}=0.03$; $H_{age}=11.28$, $p_{age}<<0.01$; $H_{sex-age}=14.53$, $p_{sex-age}<<0.001$; mAUD: $H_{sex}=5.36$, $p_{sex}=0.02$; $H_{age}=21.72$, $p_{age}<<0.001$; $H_{sex-age}=8.00$, $p_{sex-age}<0.01$; mDUD: $H_{sex}=4.91$, $p_{sex}=0.03$; $H_{age}=4.73$, $p_{age}=0.03$; $H_{sex-age}=5.61$, $p_{sex-age}=0.02$).

Conclusion: Aging causes a change in the morphology of tHb pulse waveform, making it more triangle-like. Sex is another factor differentiating the tHb pulse waveform similarity to the triangle, showing that the aged-induced changes are more pronounced in women.

Acknowledgements: The work was supported by the project Minigrants for doctoral students of the Wrocław University of Science and Technology.

Development of a Molecular Modelling and Dynamics Workflow for SGLT Membrane Transporters

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Background: Membrane proteins regulate the movement of molecules in and out of cells, playing a vital role in key biological processes such as nutrient transport, signaling, and immune response. Because their structures are difficult to determine using experimental techniques, researchers increasingly rely on computational methods to explore how these proteins are built and how they function [1]. These approaches provide valuable insights into membrane protein behavior, helping advance fields from drug discovery to molecular biology. In sodium-glucose transporters (SGLTs), MD simulations have been used to model the conformational changes of SGLTs during the transport cycle, helping to elucidate how glucose and sodium ions move across the membrane [2]. This work presents the current progress of my PhD, highlighting the development of a molecular modeling workflow for SGLT1 and SGLT2 that integrates docking, ligand parametrization, membrane embedding, and molecular dynamics simulations.

Materials and Methods: In this work, I aim to develop a comprehensive molecular modeling workflow for SGLT transporters using homology modeling with MODELLER, docking with AutoDock Vina, membrane system setup via CHARMM-GUI, and molecular dynamics simulations conducted with VMD, NAMD, and GROMACS software.

Results: I have successfully carried out docking studies using AutoDock Vina, generated ligand parameters via the CHARMM General Force Field (CGenFF), and embedded protein-ligand complexes into lipid bilayers for both equilibration and production molecular dynamics (MD) simulations. Using AutoDock Vina, I explored the binding of various inhibitors, including sotagliflozin, to SGLT1 and SGLT2, revealing key binding poses relevant to transporter function. Additionally, I constructed homology models for SGLT1, prepared membrane-embedded systems using CHARMM-GUI, and simulated their dynamics with NAMD and GROMACS. Preliminary results highlight the involvement of key residues such as Phe98, Phe453, and Gln457, which may play a significant role in the transport mechanism of SGLTs.

Conclusion: This work outlines the establishment of a robust and integrative computational workflow to investigate the structural and functional characteristics of SGLT1 and SGLT2 transporters. The findings will contribute to a deeper understanding of the mechanistic aspects of sodium-glucose transport and lay the groundwork for further refinement of structure-based drug design targeting SGLTs.

- [1] K. Goossens and H. De Winter. Molecular dynamics simulations of membrane proteins: An overview. *J. Chem. Inf. Model.*, 58(11):2193–2202, 2018.
- [2] F. B. Naughton, J. M. Rosenberg, and M. Grabe. Investigation of the transport cycle of sodium glucose transport proteins through computational simulation. *Biophys. J.*, 122(3):398a, 2023.

Synthetic α -helical PSM α 3 as an Inhibitor of Human Amyloid Aggregation

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Background: The α -helical peptide PSM α 3 belongs to the family of phenol-soluble modulins (PSMs), which are extracellular short amphipathic peptides secreted by the bacteria *Staphylococcus aureus*. PSM α 3 is of special recent interest due to its cytotoxicity and highly stable α -helical conformation, which also remains in its amyloid fibrils [1].

Materials and Methods: Synthetic PSM α 3 was evaluated for its influence on human amyloidogenic protein aggregation using a variety of experimental methods in combination with molecular modelling studies. A kinetic assay with the fluorescent dye Thioflavin T (ThT) was employed, as well as atomic force microscopy (AFM) and the attenuated total reflectance-Fourier transform infrared (ATR-FTIR) spectroscopy. Cytotoxicity and protective effects were evaluated on human endothelial cells using viability and proliferation tests.

Results: We previously demonstrated that synthetic PSM α 3, which lacks the N-terminal formyl groups seen in bacteria, does not form amyloid fibrils and maintains α -helical conformation in a monomeric form for days of incubation. We also found that synthetic PSM α 3 considerably inhibited the aggregation of particular human amyloids. For instance, PSM α 3 possesses a concentration-dependent inhibitory effect on *in vitro* fibrillation of human insulin. Molecular modelling revealed that PSM α 3 most likely inhibits the production of insulin primary nuclei by competing for residues involved in its dimerisation [2]. We have also shown recently that PSM α 3 substantially reduced human islet amyloid polypeptide (hIAPP) aggregation *in vitro*. Furthermore, synthetic PSM α 3 was not toxic to human endothelial cells, in contrast to wild-type bacterial peptide. It also protects these cells from cytotoxicity caused by hIAPP, hence enhancing their viability and rate of proliferation. Molecular modelling suggested that PSM α 3 could interact with a broader range of amyloidogenic peptides. According to predicted structures, the mechanism of PSM α 3 binding to other peptides is probably dominated by hydrophobic interactions between the PSM α 3 amino acids Phe, Leu, and Val and the partner protein's Ala, Phe, Ile, Leu, and Val.

Conclusion: Synthetic PSM α 3 acts as a selective, non-toxic inhibitor of amyloid aggregation of particular human proteins. Its anti-amyloidogenic effect depends on a target protein sequence and is highly sensitive to terminal modifications. The obtained results suggest the therapeutic potential of synthetic PSM α 3 in modulating pathological amyloid aggregation.

- [1] N. Salinas, J. P. Colletier, A. Moshe, and M. Landau. Extreme amyloid polymorphism in *Staphylococcus aureus* virulent PSM α peptides. *Nat. Commun.*, 9:1–9, 2018.
- [2] [A. Kalitnik, M. Szefczyk, A. W. Wojciechowska, J. W. Wojciechowski, M. Gąsior-Głogowska, J. Olesiak-Bañska, and M. Kotulska. Cytotoxic *Staphylococcus aureus* PSM α 3 inhibits the aggregation of human insulin *in vitro*. *Phys. Chem. Chem. Phys.*, 26:15587–15599, 2024.

Efflux Pump Inhibitors from Plant Compounds: A New Strategy to Modulate Bacterial Growth and Morphology

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Background: Antimicrobial resistance is a major global health challenge of the 21st century. It is predicted to be responsible for 10 million deaths per year worldwide by 2050 [1]. The solution may be to use antibacterial-enhancing compounds in therapy or to re-sensitize the bacteria to antibacterial compounds. The use of plant-derived efflux pump inhibitors (EPIs) can make a significant contribution to the efficacy of the therapy by affecting the ability of the bacteria to grow. This study focused on the effects of plant-derived EPIs on bacterial growth in liquid medium and the ability of cells incubated with selected inhibitors to form bacterial clusters on solid medium.

Materials and Methods: Minimum inhibitory concentrations of berberine, capsaicin, coumarin 6, curcumin, palmatine, and piperine were determined against *Proteus mirabilis*, *Escherichia coli*, *Enterococcus faecalis*, and *Bacillus cereus* using a modified resazurin assay. Subsequently, the impact of specific concentrations of EPIs on the optical density of bacterial suspensions over time was investigated in a bioreactor. Digital holotomography was used to examine EPI-induced changes in bacterial cluster growth dynamics on agar. Median refractive index values of bacterial cells, volume of structures and dry mass were analysed.

Results: Antimicrobial activity was observed for palmatine, curcumin, and berberine. Literature studies confirmed that these compounds also function as Sortase A inhibitors (SrtAIs). The addition of EPIs to the medium altered the characteristics of bacterial growth curves, particularly affecting the logarithmic phase. For *E.faecalis* cells incubated with berberine, a 53.8% decrease in the mean value of the maximum growth rate was observed. Digital holotomography revealed significant changes in cluster development characteristics on agar medium among different groups, including lack of cluster formation, slowed cell divisions, and cell elongation. The smallest increases in volume were noted for *B.cereus* (1.12 for curcumin, 1.13 for berberine, and 1.16 for palmatine), potentially due to the dual action of these compounds as EPIs and SrtAIs, leading to impaired adhesion to the agar.

Conclusion: This study showed that palmatine, berberine, and curcumin could be promising substances for antimicrobial therapy, also as a component of combination therapy. In addition, they can find applications as preservatives used in the food, pharmaceutical and cosmetic industries.

Acknowledgements: The work was partially supported by the project Minigrants for doctoral students of the Wrocław University of Science and Technology and was partially funded by National Center of Science (Grant No: 2021/41/B/ST7/04002).

- [1] K.W.K. Tang, B.C. Millar, and J.E. Moore, Antimicrobial Resistance (AMR), British Journal of Biomedical Science, 80, art. 11387, 2023.

Meibomian Gland Morphology Using Deep Learning Tools

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Introduction/Background: Meibomian glands (MG) are sebaceous glands located in the eyelid tarsus that secrete lipids forming the tear film's outer layer, reducing evaporation and preventing the ocular surface from pollutions. Morphological changes such as dropout, shortening, thinning, and tortuosity are linked to dry eye disease (DED) and aging [1]. This study aimed to analyse the relationship between MG morphology and clinical signs of DED, and to profile MG features in different patient groups.

Materials and Methods: Meibography images of the upper and lower eyelids were obtained from three groups of participants: healthy controls (H, n=42), patients diagnosed with DED (DE, n=42), and healthy patients scheduled for cataract surgery (CS, n=61), with mean ages of 62 ± 7 , 65 ± 8 , and 70 ± 6 years, respectively. All images were acquired using the Keratograph 5M (Oculus) and analysed by a pre-trained neural network with image post-processing [2]. Minor manual corrections were applied when necessary. Extracted descriptors of morphological features included number of MG, length, width, tortuosity, area and MG dropout with respect to the area of the entire eyelid tarsus. Spearman's correlation was conducted on all collected data between MG features and common clinical parameters, including DED symptoms assessed using the questionnaire (SPEED), fluorescein and non-invasive tear breakup time (FBUT and NIBUT), ocular staining (OS), and lipid layer thickness (LLT). Group comparisons between were performed using parametric or non-parametric tests depending on the distribution (Shapiro–Wilk test) and homogeneity (Levene's test). Post-hoc analyses included Tukey's or Mann–Whitney with Bonferroni correction.

Results: Correlation analysis revealed several moderate associations between MG morphology and clinical parameters ($p < 0.05$). In both eyelids, NIKBUT showed correlations with MG area ($\rho = 0.257$ upper; $\rho = 0.287$ lower) and correlations with dropout ($\rho = -0.278$ upper; $\rho = -0.325$ lower). Additionally, in the lower eyelid, FBUT was correlated with MG area ($\rho = 0.177$) and with MG dropout ($\rho = -0.188$). OS was correlated with MG dropout in upper eyelid ($\rho = 0.198$) and number of MG in lower eyelid ($\rho = -0.168$). In the upper eyelid, LLT was correlated with median MG tortuosity ($\rho = 0.174$). Statistically significant group differences were observed in several parameters. In the upper eyelid, MG area was smaller ($p = 0.014$) and dropout greater ($p = 0.015$) in DE compared to H. For the lower eyelid, median MG length was higher in CS compared to both DE and H ($p = 0.011$), while mean MG length was higher in CS only in comparison to DE ($p = 0.023$).

Conclusion: This study demonstrates that MG morphology differs between healthy individuals and those with DED. Morphological parameters of MG moderately correlated with clinical signs of tear film instability, suggesting their diagnostic potential. Deep learning-based analysis provides an objective tool for assessing MG structure and offers morphological profile of the ocular surface.

- [1] M. Y. Adil et al. Meibomian gland morphology is a sensitive early indicator of meibomian gland dysfunction. *Am. J. Ophthalmol.*, 200:16–25, 2019.
- [2] Paściak et al. Enhancing meibography-based assessment of gland morphology by utilizing an image-rotating Mask R-CNN approach. *Biomed. Signal Process. Control*, 109:108045, 2025.

Amyloidogenic Properties of a Histidine-Rich Peptides and Its Cross-Interaction with Beta-Amyloid

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Background: Protein and peptide aggregation can play a critical role in the pathogenesis of amyloidoses, including neurodegenerative diseases (NDDs) such as Alzheimer's (AD) and Parkinson's (PD) diseases, as well as non-neuropathic amyloidoses, like type II diabetes [1]. Although traditionally associated with pathology, amyloids can also fulfill essential biological functions, e.g.: participation in bacterial biofilm formation or regulation of gene expression. Increasing evidence suggests that components of the human microbiome may influence amyloid-related disorders *via* the gut-brain axis [2]. An example is the aggregation-prone and histidine-rich Hpn protein produced by *H. pylori* [3, 4]. However, its aggregation mechanisms and potential cross-interactions with host amyloids remain unclear.

Materials and Methods: The amyloidogenic properties of Hpn were investigated using a combination of methods, including: Thioflavin T (ThT) fluorescence assay, transmission electron microscopy (TEM), Fourier-transform infrared (FTIR) and circular dichroism (CD) spectroscopies [5]. Aggregation behavior was also evaluated for three selected Hpn fragments, identified by bioinformatics tools as aggregation-prone regions (APRs). In addition, the effect of C-terminal modifications (-OH or -NH₂) on amyloid formation was assessed. Preliminary ThT assays have been performed to examine the potential for cross-interaction between Hpn/Hpn(4–38) and A β .

Results: Our results showed that the Hpn(4–38) exhibits amyloidogenic properties, particularly in the C-terminal -OH form. In contrast, full-length Hpn did not form amyloid fibrils under the tested conditions, contrary to the findings reported by *R. Ge (2011)* [4]. Furthermore, peptides with C-terminal -NH₂ modifications displayed significantly reduced aggregation propensity. Preliminary ThT data suggest that Hpn may cross-interact with A β , supporting its role in host amyloid modulation.

Conclusion: These findings provide novel insights into the aggregation behavior of histidine-rich bacterial peptides and their potential to cross-interact with human amyloids. Continued research into the interplay between microbial and "pathological" proteins and peptides may advance our understanding of the microbiome's role in NDDs and contribute to the identification of new therapeutic targets.

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- [1] H. Hampel et al. The amyloid- β pathway in Alzheimer's disease. *Mol. Psychiatry*, 26(12):5481–5503, 2021.
- [2] R. P. Friedland et al. The role of microbial amyloid in neurodegeneration. *PLoS Pathog.*, 13(12): e1006654, 2017.
- [3] T. Iwasaki et al. In vitro transcytosis of *Helicobacter pylori* histidine-rich protein through gastric epithelial-like cells and the blood–brain barrier. *Biosci. Biotechnol. Biochem.*, 86(3):321–330, 2022.
- [4] R. Ge et al. Histidine-rich protein Hpn from *Helicobacter pylori* forms amyloid-like fibrils in vitro and inhibits the proliferation of gastric epithelial AGS cells. *Biochim. Biophys. Acta*, 1813(8):1422–1427, 2011.
- [5] J. A. J. Housmans et al. A guide to studying protein aggregation. *FEBS J.*, 290(2):554–583, 2023.

Deep Multiple Instance Learning for Automated Tumor Positivity Score Prediction in Non-Small Cell Lung Cancer

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Introduction/Background: Accurate assessment of TPS in NSCLC is critical for treatment planning and prognosis. However, the current method involves extensive manual labor and expertise due to the need for annotating individual slides. The aim of this study is to develop an automated deep learning approach using MIL to predict TPS at the slide level. This would reduce reliance on time-intensive manual annotations and expert resources while providing assistance in highlighting regions of high diagnostic value and offering preliminary TPS for experts' reference.

Materials and Methods: The framework consists of two key components:

- 1) A multilabel classification deep neural network trained on a publicly available dataset [1]. The architecture was chosen due to the combination of high accuracy in classifying tumor and background regions (92% and 99% respectively) and low parameter count, ensuring computational efficiency. While predicting the tissue type in each patch of an entire whole-slide image (WSI), the network effectively captures relevant histopathological features. As a result, it also functions as a low-resource embedding extractor by average-pooling activations from the final layer before the classifier. These embeddings are then passed to the next stage of the pipeline.
- 2) A lightweight multiple instance learning (MIL) attention-based model trained on 136 WSIs, which leverages embeddings from tumor-classified patches to predict the overall TPS (0-100) for the entire slide. In addition, the model generates an attention map highlighting regions of interest, enabling further analysis of the most relevant patches.

Results: The proposed framework demonstrated strong performance in slide-level TPS prediction. It achieved an average RMSE of 16.8 and Cohen's Kappa of 0.75 at the 50% threshold on the test dataset for the ensemble model, matching the results from fully supervised models [2]. By eliminating the need for manual labeling of specific regions or cells, the pipeline significantly reduces the time and effort required for TPS assessment. Finally, the model-generated data facilitates comprehensive visualization, further enhancing the explainability aspect of the system.

Conclusion: The proposed deep MIL framework demonstrates significant potential in supporting the assessment of TPS in NSCLC by providing an automated yet explainable evaluation of WSIs. Furthermore, it facilitates and streamlines future improvements and adjustments to the models by being compatible with a wide range of embedding extraction methods, depending on the available computational resources.

- [1] Y. Wang et al. MIHIC: A multiplex IHC histopathological image classification dataset for lung cancer immune microenvironment quantification. *Front. Immunol.*, 15:1334348, 2024.
- [2] M. van Eekelen et al. Comparing deep learning and pathologist quantification of cell-level PD-L1 expression in non-small cell lung cancer whole-slide images. *Sci. Rep.*, 14(7136):1–10, 2024.

Effect of Iris Colour on Speckle Noise Parameters in OCT Images and Light Scattering Parameters in Scheimplug Images of the Anterior Segment of the Eye

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Background: Corneal transparency is essential for proper optical function, as it enables accurate light focus on the retina. While traditional assessment methods, like slit-lamp examination, are subjective, modern imaging techniques such as OCT and the Scheimplug camera offer objective, quantitative evaluation of corneal densitometry [1]. However, these measurements can be influenced by various factors [2-4]. This study aimed to examine how selected anatomical features – iris colour, anterior iris tortuosity and anterior segment geometry – affect speckle noise in OCT images and light scattering in Scheimplug imaging.

Materials and Methods: The study included 31 participants, examined using Revo 80 OCT and the Corvis ST tonometer with a Scheimplug camera. Subjects were grouped by iris brightness (light/dark). Four speckle noise parameters obtained from OCT images and corresponding densitometric parameters from Scheimplug imaging were analysed. Custom MATLAB functions, based on formulas developed in earlier studies and provided by their original authors, were used to calculate these parameters [5-7]. Statistical comparisons between iris groups were performed, along with correlation analyses between speckle noise and anterior chamber geometry (ACD and CCT). The effect of iris surface tortuosity and partial correlations controlling for age, gender and iris brightness were also assessed. Finally, the consistency of densitometric results from both imaging methods was evaluated.

Results: Statistical analysis showed no significant differences in speckle noise parameters between eyes with light and dark irises ($p > 0.05$), as well as no significant correlations between speckle noise parameters and ACD and CCT. Despite being statistically insignificant, lower p-values were noted for ACD than for CCT. This may suggest a potentially greater effect of anterior chamber depth on densitometry results. Iris tortuosity also did not correlate significantly with speckle noise parameters. Including confounding factors did not change the results. However, there was a high correlation between the shape of the nasal and temporal sides of the iris ($p = 0$). In a comparative analysis of the densitometry results obtained from the Scheimplug camera and OCT, a significant correlation ($p < 0.05$) was found for only two of the four parameters analysed, suggesting the possibility of their interchangeability in further studies.

Conclusion: The study did not confirm the hypothesized effects of iris brightness and curvature on speckle noise or corneal light scattering, nor did it find significant correlations with the geometry of the anterior segment of the eye. These anatomical factors showed no notable impact on OCT or Scheimplug image parameters. Nonetheless, observed trends suggest that bigger examination database may reveal underlying relationships, underscoring the pilot nature of this study. A significant correlation between densitometric data from both imaging methods suggest their potential complementarity in clinical use. The findings support further research into better understanding of the complex interactions between the anatomy of the anterior segment of the eye and optical imaging parameters.

- [1] J. M. Schmitt, S. H. Xiang, and K. M. Yung. Speckle in optical coherence tomography. *Opt. Express*, 4(1):95–105, 1999.
- [2] A. B. Cankaya, K. Tekin, H. Kiziltoprak, S. Karahan, and P. Yilmazbas. Assessment of corneal backward light scattering in the healthy cornea and factors affecting corneal transparency. *Jpn. J. Ophthalmol.*, 62(3):335–341, 2018.
- [3] A. M. Otri, U. Fares, and M. A. Al-Aqaba. Corneal densitometry as an indicator of corneal health. *Ophthalmology*, 119(3):501–508, 2011.
- [4] N. Sorch, J. J. Rozema, S. Jongenelen, I. R. Hidalgo, and N. Zakaria. Normative values for corneal densitometry analysis by Scheimpflug optical assessment. *J. Cataract Refract. Surg.*, 39(8):1204–1210, 2013.
- [5] M. Miałdzyk, A. Consejo, and D. R. Iskander. Assessing and compensating for the confounding factors in Scheimpflug-based corneal densitometry. *Biomed. Opt. Express*, 13(12):6258, 2022.
- [6] D. A. Jesus and D. R. Iskander. Assessment of corneal properties based on statistical modeling of OCT speckle. *Biomed. Opt. Express*, 8(1):162, 2017.
- [7] M. Niemczyk and D. R. Iskander. Statistical analysis of corneal OCT speckle: a non-parametric approach. *Biomed. Opt. Express*, 12(10):6407, 2021.

Uncovering Hidden Connectivity Patterns in the Human Auditory Cortex with Computational Modelling

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Background: The exploration of sound processing in humans bridges neuroscience, psychology, and clinical science, but the precise architecture of the human auditory cortex (AC), a key brain area for sound processing, remains elusive. Due to ethical constraints, our understanding of the human AC must rely on non-invasive methods, such as magnetoencephalography (MEG). Although MEG enables the observation of neural responses, the resulting signals are difficult to interpret, as they reflect the combined activity of large populations of neurons and are often affected by a low signal-to-noise ratio. These limitations highlight the importance of developing computational models to explore and disentangle the complex mechanism underlying auditory processing.

Materials and Methods: We investigate the detailed anatomy and connectivity of the human AC through a computational modelling approach based on the hypothesis that the morphology of the MEG signal contains information about AC connectivity. In our recent work, we utilised a well-established AC model, which incorporates the core, belt, and parabelt areas, and optimised its parameters using an evolutionary algorithm (EA) to more accurately reflect the real human auditory responses. The aim of this optimisation was to capture realistic AC connectivity patterns based on empirical MEG data. The optimisation criterion focused on generating synthetic signals that closely resemble the experimental data, with connection strengths being iteratively adjusted to achieve this match. In a follow-up study, we empirically tested this strategy by applying it to MEG data collected from a group of healthy participants.

Results: A key objective of the analysis was to investigate the directional connectivity – specifically feedforward and feedback pathways – between distinct areas of the auditory cortex, which was subjected to statistical inference. We found that feedback connections were significantly stronger than feedforward connections within and between specific cortical areas.

Conclusion: Our work demonstrates how computational modelling, combined with optimisations that incorporate empirical MEG data, can offer new insights into auditory cortex connectivity. The findings point to a key role of feedback pathways in shaping auditory responses. The study highlights that parameter refinement in data-driven modelling can reveal new information about biological systems, specifically about features not directly accessible via the available *in vivo* measurement methods. Future efforts will focus on exploring alternative optimisation strategies to ensure the validity of the obtained results and to confirm that they are not influenced by a potential method-specific bias.

Other participants (oral mini-presentations)

Comparative Study of the Total Antioxidant Capacity of Selected Teas

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Background: Reactive oxygen species (ROS) are generated in the body as by-products of mitochondrial metabolism, as well as in response to inflammation, infection, and stress. Elevated levels of these reactive molecules can lead to oxidative stress, which damages cellular components such as membranes, proteins, lipids, and nucleic acids. Certain types of tea may contain antioxidants capable of neutralizing ROS [1, 2].

Materials and Methods: The ABTS radical cation decolorization method was employed to assess total antioxidant capacity (TAC) selected types of tea, namely black, green, white, and red (Rooibos) teas. To compare the TAC coefficient values between the studied groups, a one-way Analysis of Variance (ANOVA) was employed. Subsequently, if significant differences were found, post-hoc comparisons were conducted using Tukey's test to identify specific differences between group pairs.

Results: The highest TAC values were observed in black tea, followed by green, white, and, lastly, red tea. Statistical analysis using one-way ANOVA followed by Tukey's post hoc test confirmed significant differences in TAC values between the individual types of tea, confirming that tea type affects antioxidant potential.

Conclusion: Our results demonstrate that teas vary in their antioxidant potential, offering insights that may help guide dietary choices to combat oxidative stress.

- [1] L. A. Pham-Huy et al. Free radicals, antioxidants in disease and health. *Int J Biomed Sci*, 4(2):89–96, 2008.
- [2] G. Pizzino et al. Oxidative Stress: Harms and Benefits for Human Health. *Oxid Med Cell Longev*, 8416763, 2017.

Bioinformatics Analysis of the Impact of the Gut-brain Axis on Neurodegenerative Diseases

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Background: The gut–brain axis represents a complex communication system linking the gastrointestinal tract with the central nervous system, integrating neuronal, immunological, and hormonal signals [1]. In recent years, there has been growing interest in its role in the pathogenesis of neurodegenerative diseases, such as Parkinson’s disease and Alzheimer’s disease [2]. The aim of this study is to present the mechanisms by which disturbances in the gut microbiota (dysbiosis) and its metabolic products may influence the brain and promote neurotoxic processes. Particular attention is given to the phenomenon of cross-seeding between bacterial and human amyloids, which may initiate or accelerate the pathological aggregation of proteins such as α -synuclein and β -amyloid [3].

Materials and Methods: The research section includes a bioinformatic analysis of bacterial proteomes enriched in the gut microbiota of patients with neurodegenerative diseases, identifying amyloidogenic sequences present in their proteins.

Results: The results led to the selection of candidates for further functional and structural studies, some of which exhibited known aggregation-prone motifs. The literature data, combined with the bioinformatic findings, suggest that the gut may be a primary site for the initiation of pathological protein aggregation, redefining the traditional view of neurodegeneration as a solely neurological condition.

Conclusion: This insight opens the possibility of developing novel, personalized therapeutic strategies based on microbiome modulation – including probiotics, fecal microbiota transplantation, and pharmacological interventions targeting specific bacterial pathways. Recognizing the impact of the gut microbiota on brain health creates an opportunity for the advancement of precise diagnostic and therapeutic tools in future medicine [4].

- [1] C. Yuan, Y. He, K. Xie, L. Feng, S. Gao, and L. Cai. Review of microbiota gut brain axis and innate immunity in inflammatory and infective diseases. *Frontiers in Cellular and Infection Microbiology*, 13, 2023.
- [2] S. Khatoon, N. Kalam, S. Rashid, and G. Bano. Effects of gut microbiota on neurodegenerative diseases. *Frontiers in Aging Neuroscience*, 15, 2023.
- [3] T. Sampson. Microbial amyloids in neurodegenerative amyloid diseases. *The FEBS Journal*, 292(6):1265–1281, 2023.
- [4] F. Taghizadeh Ghassab, F. Shamlou Mahmoudi, R. Taheri Tinjani, A. Emami Meibodi, M.R. Zali, and A. Yade gar. Probiotics and the microbiota-gut-brain axis in neurodegeneration: Beneficial effects and mechanistic insights. *Life Sciences*, 350:122748, 2024.

Non-Contact and Label-Free Evaluation of the Strategy Against Surface-Adhering Microorganisms

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Background: 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. Antifouling effects can be achieved through increased surface hydrophobicity and roughness, which hinder microbial adhesion and interfere with cellular structures like bacterial fimbriae. Nanoparticles are often used to engineer such surface properties.

Materials and Methods: Coatings were prepared using silica colloids in two molar proportions (R20 and R50), indicating different silica-to-solvent ratios, as matrices to suspend multiwalled carbon nanotubes (MWCNTs) and halloysite nanoclay. Nanomaterials were dispersed in 1 ml of colloid with Triton X-100, mixed, and applied (200 μ l) to glass slides. A total of 110 samples were prepared, including standard coatings (n=40), dual-layer coatings with MWCNTs applied over dried colloid (20 $\times$ R20, 10 $\times$ R50), and sonicated MWCNT-R20 samples (n=20), plus colloid-only controls (10 $\times$ R20, 10 $\times$ R50). Surface topography of the coatings was imaged using optical coherence tomography (OCT). Cross-sectional scans were analyzed using a custom script; edge detection and signal processing were used to calculate classical roughness (Ra), with roughness analyzed across macro-, micro-, and nanoscale frequency bands. Wettability was evaluated via static contact angle measurements using side-view photographs of water droplets deposited on the surface. Images were captured in series using a fixed camera setup immediately after the droplet application.

Results: Significant increases in water contact angle were observed for coatings with MWCNTs, particularly in R20 formulations with double-layer application and sonication, indicating improved hydrophobicity. These variants demonstrated statistically significant differences compared to control samples. The increase in contact angle was consistent with elevated surface roughness, especially in the high-frequency range. In contrast, coatings incorporating halloysite nanoclay did not lead to improved hydrophobicity, and samples based on the R50 colloid generally showed lower contact angles than those based on R20.

Conclusion: The results demonstrate that MWCNTs can be effectively used to engineer hydrophobic surface coatings. Optimized application methods, like sonication or double-layer deposition, led to improved results. This suggests that nanostructuring and proper formulation of colloidal matrices can be a viable strategy for designing surfaces with tailored wetting properties. In contrast, not all nanomaterials provided the desired effect, highlighting the importance of material choice and surface architecture.

- [1] Antimicrobial Resistance Collaborators. Global burden of bacterial antimicrobial resistance 1990–2021: a systematic analysis with forecasts to 2050. *Lancet*, 404(10459):1199–1226, 2024.

CH-Acidity of Heterocycles in Gas and Solution Phases: A Quantum Chemical Approach

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Background: Heterocyclic compounds are widely used in pharmacology, materials science, and organic synthesis. A key physicochemical property influencing their reactivity is CH-acidity, which is particularly important in reactions such as deprotonation and metalation. Due to the experimental challenges in determining CH-acidity constants, quantum chemical methods offer a promising alternative for their accurate prediction.

Materials and Methods: Quantum chemical calculations were performed using the Gaussian 09W software. Composite methods (G3, G4, G3B3) were applied for gas-phase acidity calculations, while density functional theory (DFT, B3LYP/6-311+G(d,p)) in combination with continuum solvent models (SMD, IEFPCM, CPCM, SCI-PCM) was used for acidity estimation in tetrahydrofuran solution. Isodesmic reactions and thermodynamic cycles were utilized to calculate pKa values [1].

Results: Quantum-chemical calculations of CH-acidity for a series of heterocyclic compounds were performed using Gaussian 09, employing composite methods (G3, G4, G3B3) for gas-phase acidity and DFT-B3LYP with 6-31G(d) and 6-311+G(d,p) basis sets for solution-phase calculations in THF. The SMD solvent model provided the most accurate pKa values compared to IEFPCM, SCI-PCM, and CPCM, with an average deviation of ≈ 1.43 pKa units from experimental data. Geometry optimization in solution improved accuracy for most compounds, reducing the mean absolute error to 1.30 pKa units, though 1-methylpyrrole showed a notable deviation. Furan and 1-methylimidazole as reference compounds yielded comparable results, with furan selected for consistency. Benzoxazole exhibited the highest CH-acidity, while 1-(dimethylamino)pyrrole had the lowest.

Conclusion:

The optimal methodology for calculating CH-acidity constants involves G3B3 for gas-phase Gibbs free energy, DFT-B3LYP/6-31G(d) for solution geometry optimization, and DFT-B3LYP/6-311+G(d,p) with the SMD model for solvation energy, using furan as the reference compound. This approach yields pKa values in good agreement with experimental data, except for 1-methylpyrrole, suggesting the need for alternative functionals or atomic radii. The study highlights the SMD model's superiority for low-dielectric solvents like THF and underscores the importance of solution-phase geometry optimization for enhancing calculation accuracy.

- [1] V. E. Matulis, Y. S. Halauko, O. A. Ivashkevich, and P. N. Gaponik. CH acidity of five-membered nitrogen-containing heterocycles: DFT investigation. *J. Mol. Struct. THEOCHEM*, 909(1):19–24, 2009.

Joint Analysis of Slow Waves and Pulse Waveform of Intracranial Pressure in Traumatic Brain Injury Patients

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Introduction. The intracranial pressure (ICP) signal contains several components, including slow waves related to slow vascular activity and the pulse waveform which represents changes over a single cardiac cycle. These components provide important information about the condition of patients with traumatic brain injury (TBI), specifically the state of cerebral autoregulation and cerebral compliance. The aim of this study was to examine the relationship between parameters related to slow waves and the pulse waveform, as well as their prognostic value after TBI.

Methods. The study analyzed ICP and arterial blood pressure (ABP) recordings from 187 TBI patients from the CENTER-TBI database. The analyzed parameters included: slow wave power assessed using power spectral density analysis in the 0.005-0.05 Hz range, pressure reactivity index (PRx) calculated as the correlation coefficient between slow changes in ICP and ABP, and the pulse shape index (PSI) based on automatic classification of ICP pulse waveforms. The study assessed Spearman correlations between the parameters as well as group differences between surviving and deceased patients at discharge from the intensive care unit (ICU) and those with poor and good outcome 6 months after injury using Mann-Whitney U test (significance level 0.05).

Results. The strongest correlation was observed between PSI (median=2.38, IQR: 0.67) and age (median=47.5, IQR: 24.75) ($r=0.50$, $p<0.0001$). PRx showed significant correlations with age ($r=0.28$, $p=0.0001$) and PSI ($r=0.25$, $p=0.0007$). Slow wave power showed no statistically significant correlations with any of the studied variables. Patients who did not survive the ICU stay were characterized by higher PRx values (median=0.24, IQR: 0.13 vs median=-0.00 for survivors; $p<0.001$) but lower PSI values (median=2.29, IQR: 0.67 vs median=3.07, IQR: 0.64 for survivors; $p=0.0004$). In the assessment of 6-month neurological outcome, poor outcome was associated with higher PRx values (median=0.03, IQR: 0.21 vs median=-0.01 for good outcome; $p=0.0141$) and lower PSI values (median=2.29, IQR: 0.68 vs median=2.47, IQR: 0.69 for good outcome; $p=0.0305$). Slow wave power showed statistically significant differences only in the context of 6-month neurological outcome (median=0.61, IQR: 0.80 for poor outcome vs median=0.47, IQR: 0.69 for good outcome; $p=0.0409$).

Conclusions. The study demonstrated a moderate but significant relationship between indices corresponding to the autoregulatory and pulsatile components of the ICP signal. As those components are overlaid in the time domain, their interrelationship may influence the results of assessment of the state of the cerebrospinal space in TBI patients. Further analysis is required to determine causal relationships between changes in slow wave activity and the pulse waveform.

Electrochemical Immunosensor Based on Biocompatible Protein-Based Nanofibers for Cortisol Detection

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Background: Chronic psychological stress has become a global health concern, and is linked to conditions such as cardiovascular diseases and mental health disorders [1]. Cortisol, a key biomarker of stress, necessitates real-time monitoring for effective stress assessment [1,2]. Traditional diagnostic tools are time-consuming and requires trained personnel, making biosensors a promising alternative for fast and accessible diagnostic tools [2]. Electrochemical immunosensors based on nanomaterials are increasingly used for cortisol detection due to their unique properties compared to bulk materials, enhancing overall sensor performance [1,2]. In particular, protein-based electrospun nanofibers offer excellent biocompatibility along with their superior surface-to-volume ratio, enabling improved antibody immobilization [3]. In this study, a novel electrochemical immunosensor was developed by directly integrating protein into electrospun nanofibers, enabling the rapid fabrication of a simplified platform for cortisol detection.

Materials and Methods: The immunosensor platform was made of a platinum electrode modified through a two-step process: (1) deposition of hybrid protein-polymer nanofibers *via* electrospinning, and (2) surface functionalization through antibody immobilization followed by bovine serum albumin blocking to prevent non-specific binding [4]. Morphological characterization was done *via* optical microscopy (OM) and transmission electron microscopy (TEM). Electrochemical characterization *via* cyclic voltammetry (CV) and differential pulse voltammetry (DPV) was performed to determine key performance parameters such as stability, selectivity, sensitivity, limit of detection, and linearity. The sensor was also evaluated in human serum to assess real-sample application.

Results: Successful nanofiber synthesis and subsequent modification steps were confirmed by OM and TEM, respectively. The immunosensor exhibited good stability, selectivity, sensitivity, and linearity in the range of 0.1 – 15 μM , with a low limit of detection equal to 0.01 μM . It also showed promising performance in human serum, indicating potential for clinical applications.

Conclusion: The fabricated immunosensor exhibited good analytical performance and offers a fast and cost-effective platform for the clinical determination of cortisol, with potential for future point-of-care applications.

- [1] Z. Li, D. Luo, Y. Zhang, X. Niu, and H. Liu. Smart health monitoring: review of electrochemical biosensors for cortisol monitoring. *Adv. Healthc. Mater.*, 14(11):e2404454, 2025.
- [2] C.-E. Karachaliou et al. Cortisol immunosensors: a literature review. *Biosensors*, 13(2):285, 2023.
- [3] A. Kakoria and S. Sinha-Ray. A review on biopolymer-based fibers via electrospinning and solution blowing and their applications. *Fibers*, 6(3):45, 2018.
- [4] B. Sun et al. Investigate electrochemical immunosensor of cortisol based on gold nanoparticles/magnetic functionalized reduced graphene oxide. *Biosens. Bioelectron.*, 88:55–62, 2017.

Using Deep Canonical Correlation Analysis to Reveal Relationship Between Intracranial Pressure and Arterial Blood Pressure in Traumatic Subarachnoid Haemorrhage Patients

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Background: Traumatic Subarachnoid Haemorrhage (tSAH) is a bleeding into the subarachnoid space caused by a traumatic brain injury (TBI). It can lead to life-threatening dysfunction of the autonomic nervous system. Severe tSAH is linked to impairment of respiratory centers leading to acute respiratory distress in 48 hours post-admission [1]. The severity of tSAH is determined using Fisher scale on computed tomography scans. The link between severity of tSAH and impaired cerebral autoregulation is unclear and could be described by Deep Canonical Correlation Analysis (DCCA), a technique which measures nonlinear associations between two multivariate sets of variables [2].

Materials and Methods: ICP and ABP recordings from 125 TBI patients from the CENTER-TBI high-resolution sub-study were retrospectively analysed. The median age of the patients was 51 years. Patients were divided into two groups: present tSAH (n=111) and absent tSAH (n=14). A severe haemorrhage was defined as a Fisher grade between 3 and 4 (n=47), while a moderate haemorrhage was defined as a Fisher grade between 1 and 2 (n=78). In both cases, the larger group of patients was split into training and testing sets, while the smaller group was used for additional testing. Signals were transformed using DCCA and the first five canonical components were analysed. The National Science Centre (UMO-2022/47/D/ST7/00229) supported this study.

Results: The first five canonical correlations were higher in the absent tSAH group (0.99, 0.89, 0.83, 0.46, 0.31) than in the present tSAH group (0.69, 0.41, 0.29, 0.23, 0.12). There were no meaningful differences between a severe haemorrhage (0.72, 0.45, 0.36, 0.29, 0.07) and a moderate haemorrhage (0.77, 0.59, 0.43, 0.30, 0.02) groups.

Conclusion: Differences in the relationship between ICP and ABP in the absent-tSAH and present-tSAH groups may indicate impaired autoregulation in the latter. No differences between severe and moderate haemorrhage groups were observed, which may suggest a similar influence of haemorrhage severity on cerebral autoregulation. The main limitation of this study was an unbalanced division of patients based on the presence of tSAH. Further study is needed to investigate the relationship between ICP and ABP and the mechanism of the haemorrhage.

- [1] M. Li, R. Wang, Q. X. Fang, Y. X. He, Y. W. Shi, S. N. Ge, R. N. Ma, and Y. Qu. Association between Traumatic Subarachnoid Hemorrhage and Acute Respiratory Failure in Moderate-to-Severe Traumatic Brain Injury Patients. *Journal of clinical medicine*, 11(14): 3995, 2022.
- [2] G. Andrew, R. Arora, J. Bilmes, K. Livescu. Deep Canonical Correlation Analysis. *Proc. of the 30th Intl. Conference on Machine Learning*, 2013.

Variability of Gait Parameters During Treadmill Walking

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Background: Gait variability reflects the natural fluctuations in walking patterns and is considered an important indicator of motor control and stability. Previous studies have shown that changes in walking speed can influence both the mean values and variability of gait parameters such as stride length (SL), stride time (ST), and stride speed (SS). Understanding how treadmill velocity affects these parameters provides insight into locomotor control mechanisms and may have applications in clinical assessment and rehabilitation.

Materials and Methods: Ten healthy subjects (3 males, 7 females) from Wrocław University of Science and Technology participated in this study. Marker coordinates were recorded on the lateral ankles using the OptiTrack motion capture system. Stride parameters – including ST, SL, and SS – were calculated based on the anteroposterior ankle displacement. Additionally, the variances of these gait parameters were computed. The effect of treadmill velocity on both the mean and variance of stride parameters was evaluated using either ANOVA or the Kruskal–Wallis test, depending on the normality of the data.

Results: Figure 1 presents boxplots of gait parameter variances across three treadmill velocities. Statistical analysis showed that variance significantly depended on velocity for all parameters. Variance of SL decreased with increasing speed, with significant differences observed between all velocity groups. A similar but less pronounced decreasing trend was found for stride speed SS variance. For ST, variance was significantly lower at the two higher speeds compared to the lowest speed.

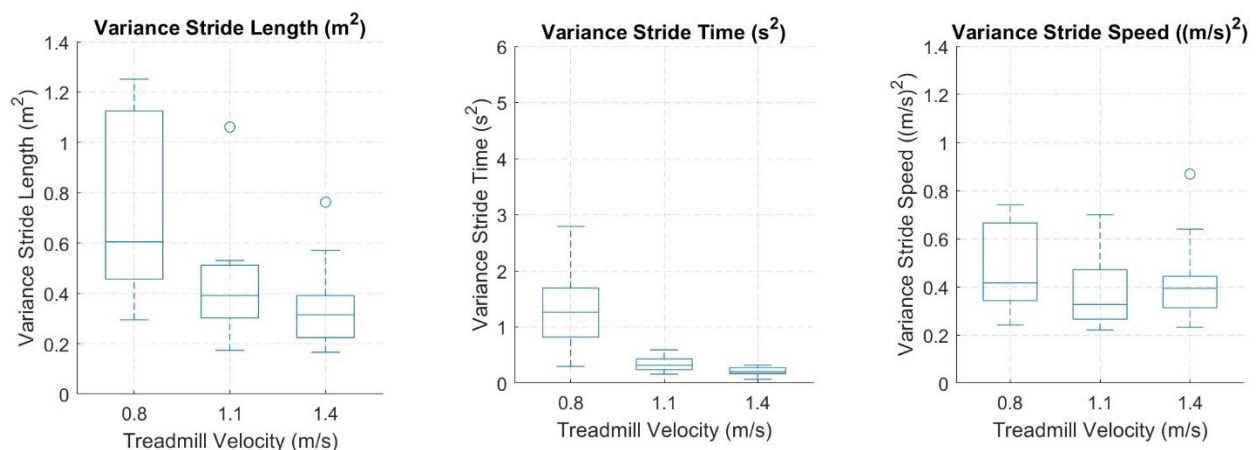


Figure 1. Boxplots of gait parameters across three treadmill speeds. Each boxplot represents the distribution of individual subject means for the respective velocity. Note: variances are scaled by a factor of 1000 for clarity.

Conclusion: The variability of gait parameters is influenced by treadmill velocity. Specifically, stride length and stride speed variances decrease as walking speed increases, suggesting more consistent gait patterns at higher speeds. Stride time variance also decreases, but only significantly between the lowest and higher speeds. These findings highlight the effect of locomotion speed on gait stability and could inform rehabilitation or training protocols that aim to improve gait consistency.

Storage-Related In Vitro Aging: Effects on the Biophysical and Rheological Properties of Human Erythrocytes

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Background: Gradual biophysical changes generated during the aging process affect the stability and viability of erythrocyte storage *in vitro*. The study investigates these changes, especially the rheological properties of aging erythrocytes. Rheological studies aim to reveal changes in deformability, aggregation, and viscosity, showing that older erythrocytes become less deformable and may aggregate differently, potentially affecting microcirculation. These studies were combined with analyses of osmotic fragility, morphology, and hemolysis. A comprehensive assessment of these parameters provides insight into how erythrocyte aging affects their ability to perform their functions.

Materials and Methods: The study investigated time-dependent changes in stored red blood cells by examining samples kept in SAGM for 1, 2, and 4 weeks. Osmotic fragility was assessed in a range of NaCl concentrations. Erythrocyte morphology was evaluated using a Mindray BC-2800 and microscopy, with AI-powered analysis from the Redtell application. Hemolysis was quantified through spectrophotometric measurements. The rheological properties of the stored erythrocytes were determined using a Laser-assisted Optical Rotational Cell Analyzer (LORRCA). Additionally, red blood cell populations were fractionated based on density by performing density gradient centrifugation using a Percoll solution.

Results: The study's analysis highlighted a significant relationship between the duration of *in vitro* storage and erythrocyte osmotic fragility, showing that older cells shift toward higher NaCl concentrations. This alteration in osmotic fragility occurred alongside morphological changes like increased MCV and echinocytes. We also observed a progressive increase in free hemoglobin and cell fragmentation over time.

Conclusion: Presented study clearly shows that longer red blood cell (RBC) storage significantly impacts their quality. Intriguingly, the number of cells analyzed influenced the observed population characteristics, and rheological measurements via LORRCA revealed significant differences in deformability across erythrocyte subpopulations. These results strongly show the need for innovative strategies to address red blood cell storage lesions.

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Evaluation of the Influence of Selected Environmental Factors on the Dehydration Process of Hydrogel Matrices

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Background: Hydrogels are widely utilized in biomedical applications such as wound dressings, drug delivery systems, and contact lenses due to their biocompatibility and tunable physicochemical properties. However, their stability and structural integrity under external stimuli, such as ultraviolet (UV) radiation and elevated temperature, remain critical for performance in real-world applications. This study aimed to assess the structural and functional stability of various hydrogel materials when exposed to UV light and temperature variations.

Materials and Methods: Five types of contact lenses, three custom-synthesized alginate-based hydrogels, and one commercial hydrogel dressing (Purilon) were examined. Fresh contact lenses were irradiated with UV (Sunone UV LED 36W lamp) for 3, 5, and 7 minutes, followed by ATR-FTIR spectral analysis. For thermal testing, lenses were placed on a temperature-controlled GladiATR accessory (Nicolet 6700 FT-IR) and analyzed after 5 minutes at specific temperatures. Hydrogels were synthesized using sodium alginate and 0.3 M solutions of CaCl₂, CoCl₂ and CuSO₄. These spheres were also exposed to UV and analyzed via ATR-FTIR before and after exposure. Temperature effects were studied after 1, 3, and 5 minutes at 22–65 °C. Dehydration was assessed by monitoring IR absorption bands at ~3400 cm⁻¹ (O–H) and ~1640 cm⁻¹ (H–O–H).

Results: Contact lenses showed consistent spectral changes upon UV exposure and thermal treatment. A progressive decrease in peak intensity and area in the O–H and H–O–H bands indicated water loss. Notably, these bands yielded slightly different dehydration percentages due to differences in vibrational sensitivity: the O–H stretching band is more responsive to hydrogen bonding changes, while the H–O–H bending band reflects the presence of free or weakly bound water [1]. Among the tested lenses, silicone hydrogel-based types exhibited slightly better resistance to dehydration under thermal conditions, while conventional hydrogel lenses were more susceptible, particularly after 7 minutes of UV exposure. Spectral shifts in both bands suggest structural changes in the hydrogen-bonding network due to water loss. Alginate based hydrogels were far more resistive to high temperatures than polymer-based contact lenses. Additionally shifts in polymer-related bands indicated both degradation and formation of physical crosslinks in different lenses.

Conclusion: The results indicate that ATR-FTIR is a semi-reliable tool for assessing dehydration and molecular structure changes in soft biomaterials. Contact lenses vary in their stability depending on material composition; silicone hydrogel lenses perform better under thermal stress. UV and thermal exposure cause measurable changes in hydrophilic properties, suggesting potential implications for comfort and performance during wear.

- [1] V. Enev, P. Sedláček, S. Jarábková, T. Velcer, and M. Pekař. ATR-FTIR spectroscopy and thermogravimetry characterization of water in polyelectrolyte-surfactant hydrogels. *Colloids Surf. A Physicochem. Eng. Asp.*, 575:1–9, 2019.