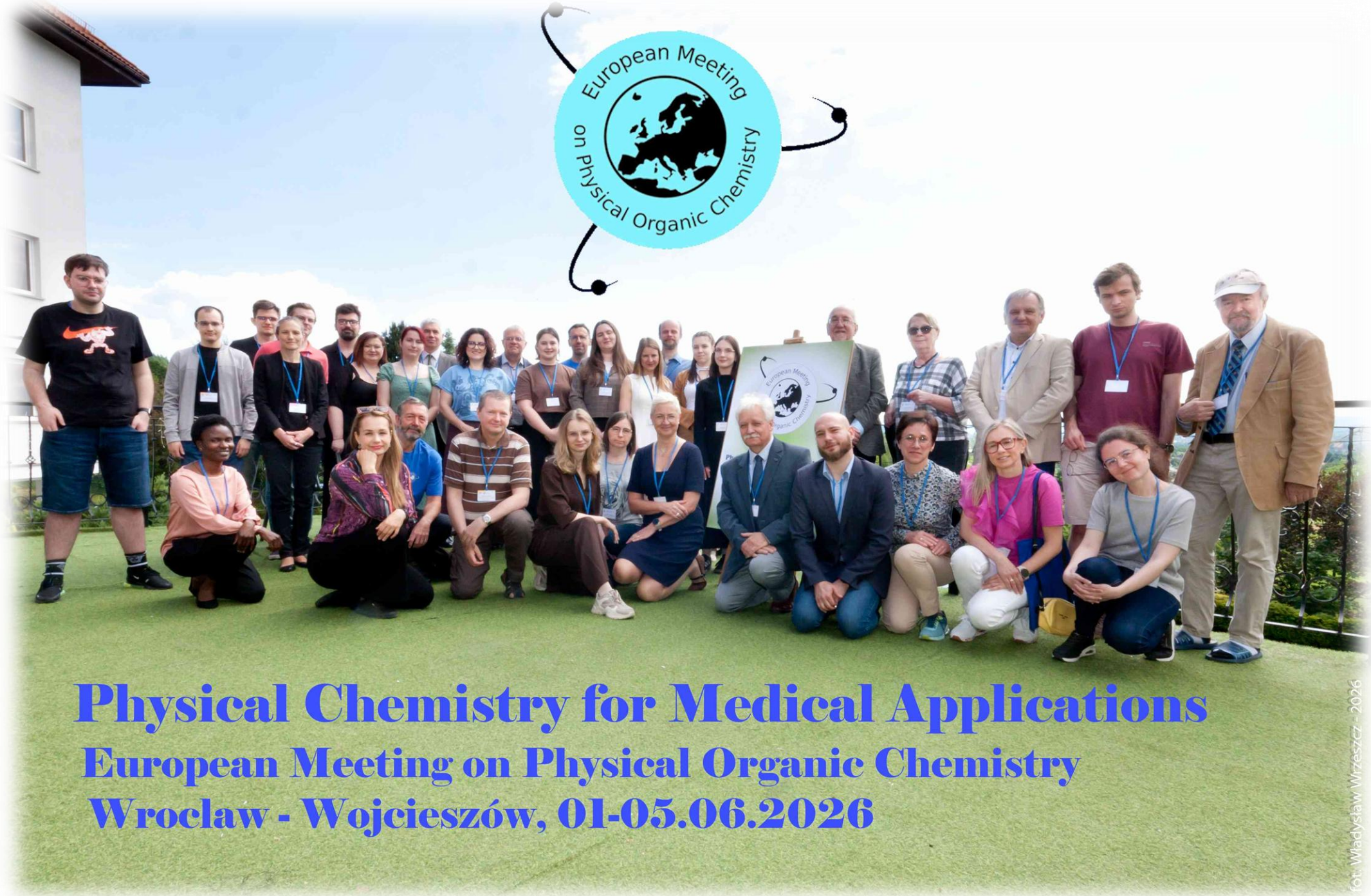
European Meeting
on Physical Organic Chemistry
Physical Chemistry for Medical Applications
European Meeting on Physical Organic Chemistry
Wroclaw - Wojcieszów, 01-05.06.2026
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Plenary lectures and oral presentations

Prof. dr hab. Małgorzata Barańska

Challenges in spectroscopic imaging of cells: an analytical and physical chemistry perspective

Dr hab. Sylwester Mazurek

Discriminant analysis of seminal plasma samples using FTIR-ATR spectroscopy

Dr Barbara Zupančič

Identifying diabetes-related biochemical changes in human tissues using infrared spectroscopy

Dr hab. Zbigniew Galewski, Prof. UWr

Liquid crystals in medical applications

Dr Amanda Bartkowiak

SGLT 2 inhibition improves red blood cell oxygenation and elasticity: another positive effect of flozin therapy

Dr Iwona Płowaś-Korus

Osmolityes in humans - biological significance and clinical implications

Prof. dr hab. Kazimierz Orzechowski

Dielectric methods in assessing the cleanliness of surgical margins in breast cancer

Dr hab. Andrzej Teisseyre

The inhibitory effects of selected flavonoids on the activity of voltage-gated potassium channels Kv1.3

Dr Marta Gordel-Wójcik

Ultrafast excited-state dynamics in trimethoxysilylazachalcone-functionalized colloidal gold nanoshells

Dr Justyna Krupa

UV-induced chemistry in interstellar ice analogues: from simple molecules to complex systems

Prof. dr hab. Teobald Kupka

Toward accurate NMR shieldings in fluoromethanes

Prof. dr hab. Adam Proń

Donor–acceptor macromolecular organic semiconductors as precursors of novel electronic, electrochromic, and photoelectrocatalytic materials

dr hab. Barbara Hachuła, prof. UŚ

Rigid cage, variable nature: spectroscopic study of phase transition in adamantane-based active pharmaceutical ingredients

Prof. Poul Erik Hansen

Drugs, natural products and hydrogen bonding (online lecture)

Dr hab. inż. Rafał Szabla

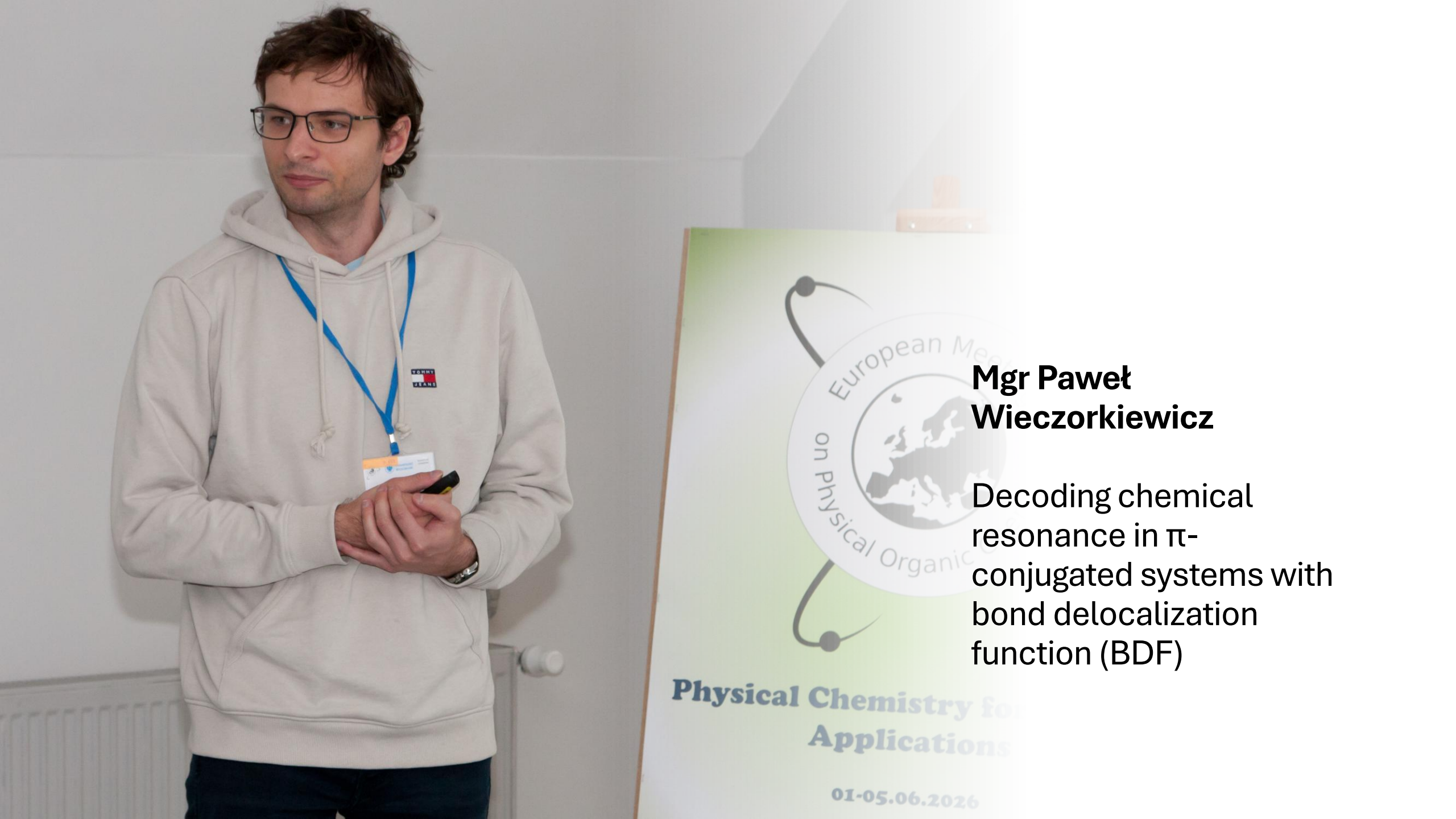
Machine learning in RNA atomistic simulations

Dr Michał Pocheć

Machine learning in RNA atomistic simulations

Dr hab. Dawid Dębowski, prof. UG

From molecular structure to biological activity: Novel sulfonamide derivatives



Mgr Paweł Wieczorkiewicz

Decoding chemical resonance in π-conjugated systems with bond delocalization function (BDF)

Mgr Barbara Lech

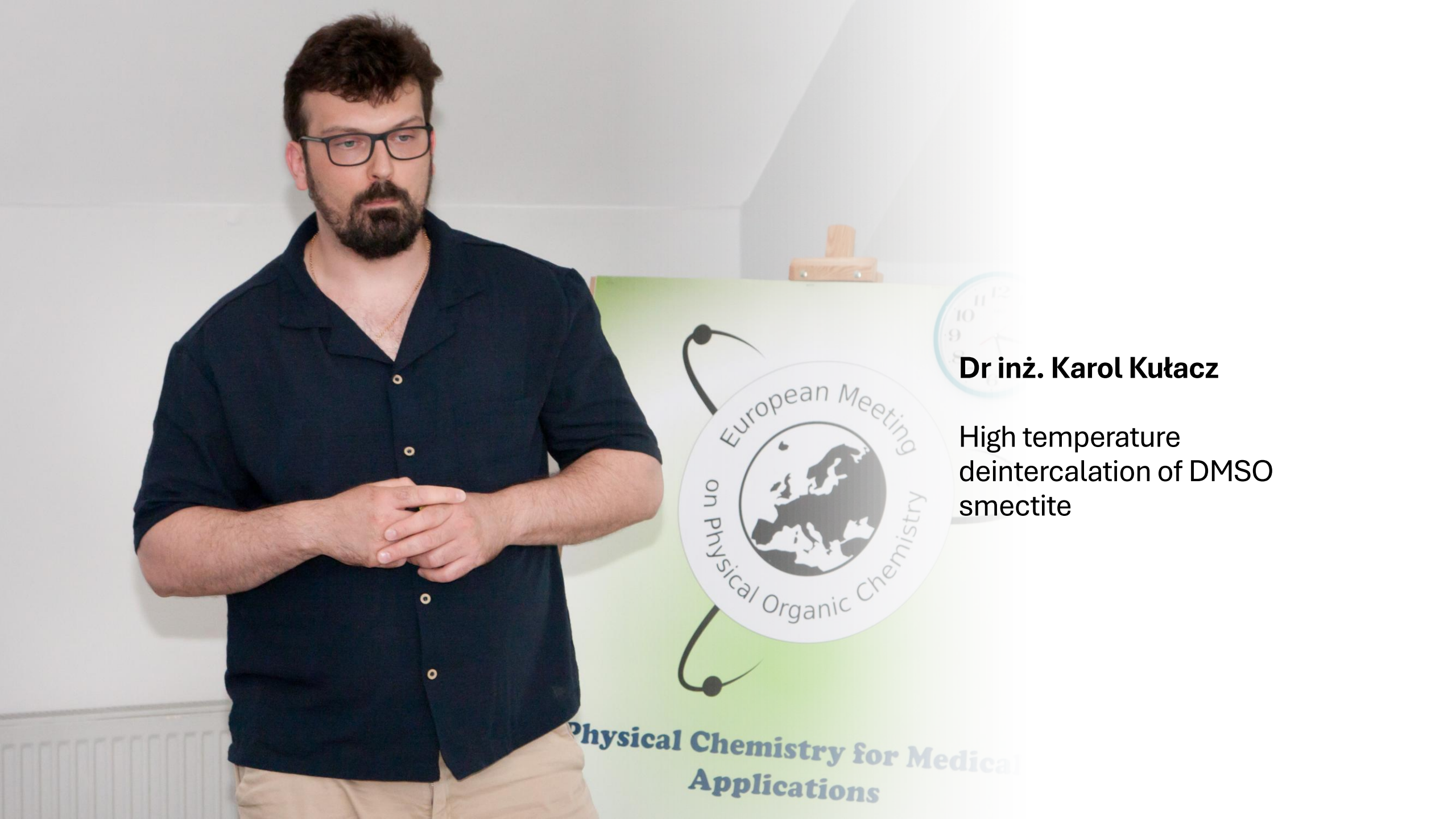
Computational insights into the role of 2-thiouracil in RNA self-replication

Dr Kamil Wojtkowiak

pH dependence of protoribosomal RNA conformational flexibility: MD simulation parameters benchmark and preliminary results

Prof. dr hab. Piotr Cysewski

Solubility advantage of (natural) deep eutectic solvents: insight from measurements, quantum chemistry and machine learning



Dr inż. Karol Kułacz

High temperature deintercalation of DMSO smectite

Prof. Mirosław Jabłoński

A thorough Systematic conformational study of an experimentally known lantern-like superphane

Prof. Vlada Pashynska

Nanocomposites of MoS2 with anticancer drugs for drug delivery: experimental and theoretical characterization

Mgr Natalia Makieieva

Towards the structure-activity correlation for selected thiosulfonates - spectroscopic studies and molecular modelling

Mgr Patrycja Piękoś

Meso-benzodioxole-BODIPY as pH-sensitive fluorophores

Poster session

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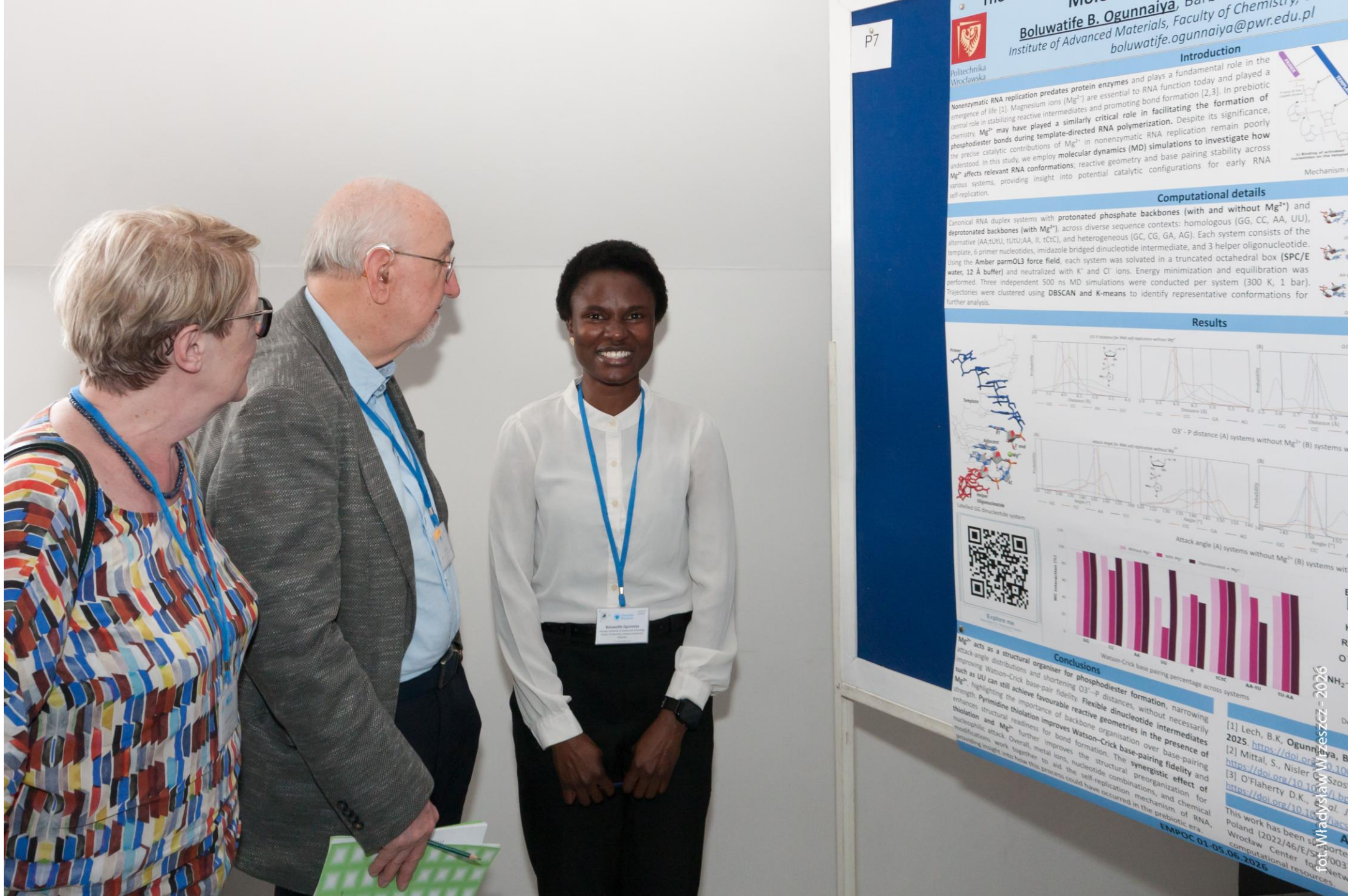
P7
Boluwatife B. Ogunnaiya
Institute of Advanced Materials, Faculty of Chemistry
boluwatife.ogunnaiya@pwr.edu.pl
Politechnika Wrocławska
Introduction
Computational details
Results
Conclusions
EMPOC 01-05.06.2026
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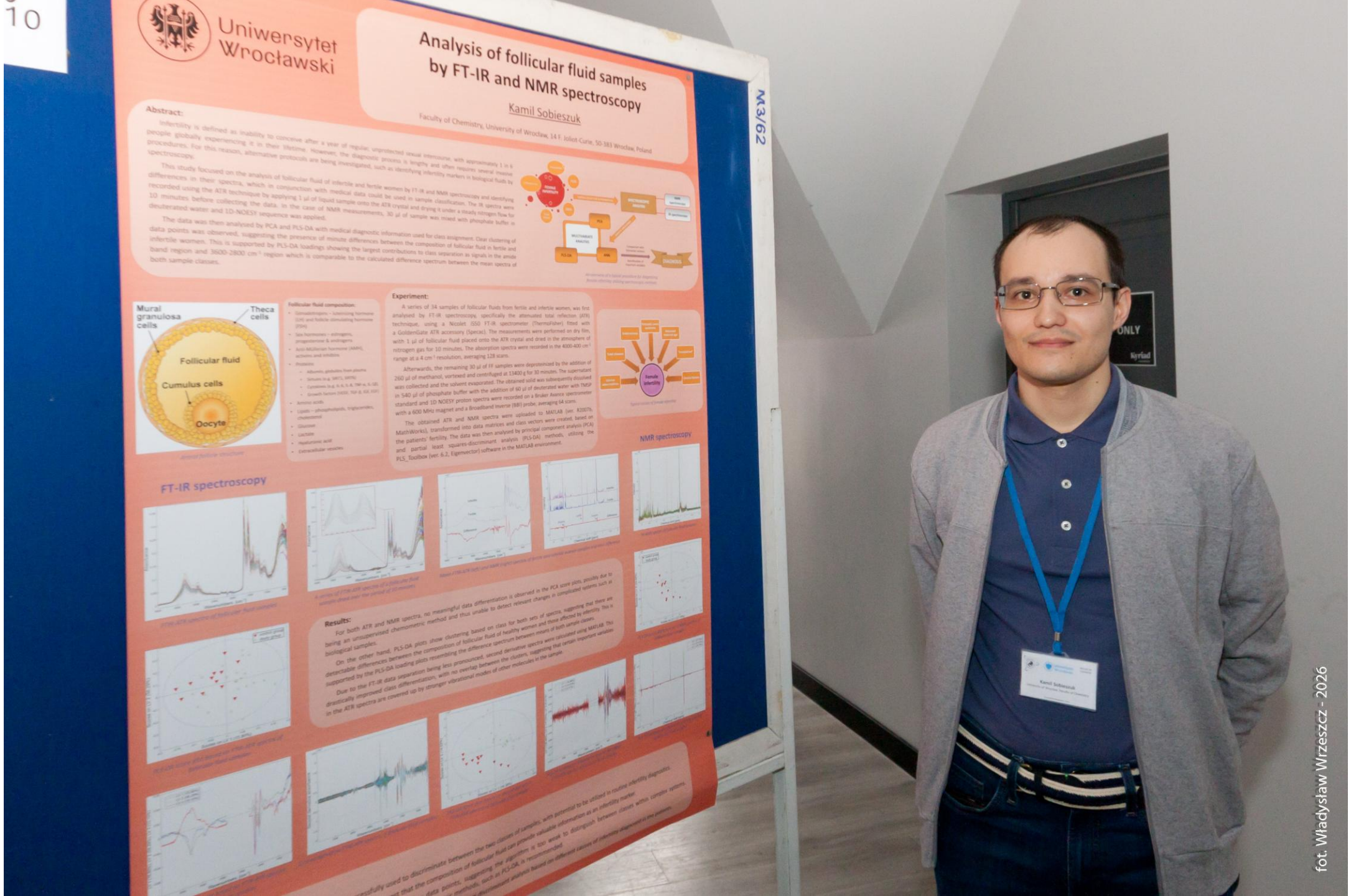
Uniwersytet Wrocławski
Analysis of follicular fluid samples by FT-IR and NMR spectroscopy
Kamil Sobieszuk
Faculty of Chemistry, University of Wrocław, 14 F. Joliot-Curie, 50-383 Wrocław, Poland
Abstract:
Infertility is defined as inability to conceive after a year of regular, unprotected sexual intercourse, with approximately 1 in 6 people globally experiencing it in their lifetime. However, the diagnostic process is lengthy and often requires several invasive procedures. For this reason, alternative protocols are being investigated, such as identifying infertility markers in biological fluids by spectroscopy.
This study focused on the analysis of follicular fluid of infertile and fertile women by FT-IR and NMR spectroscopy and identifying differences in their spectra, which in conjunction with medical data could be used in sample classification. The IR spectra were recorded using the ATR technique by applying 1 µl of liquid sample onto the ATR crystal and drying it under a steady nitrogen flow for 10 minutes before collecting the data. In the case of NMR measurements, 30 µl of sample was mixed with phosphate buffer in deuterated water and 1D-NOESY sequence was applied.
The data was then analysed by PCA and PLS-DA with medical diagnostic information used for class assignment. Clear clustering of data points was observed, suggesting the presence of minute differences between the composition of follicular fluid in fertile and infertile women. This is supported by PLS-DA loadings showing the largest contributions to class separation as signals in the amide band region and 3600-2800 cm⁻¹ region which is comparable to the calculated difference spectrum between the mean spectra of both sample classes.
Mural granulosa cells
Theca cells
Follicular fluid
Cumulus cells
Oocyte
Follicular fluid composition:
Experiment:
A series of 34 samples of follicular fluids from fertile and infertile women, was first analysed by FT-IR spectroscopy, specifically the attenuated total reflection (ATR) technique, using a Nicolet iS50 FT-IR spectrometer (ThermoFisher) fitted with a GoldenGate ATR accessory (Specac). The measurements were performed on dry film, with 1 µl of follicular fluid placed onto the ATR crystal and dried in the atmosphere of nitrogen gas for 10 minutes. The absorption spectra were recorded in the 4000-400 cm⁻¹ range at a 4 cm⁻¹ resolution, averaging 128 scans.
Afterwards, the remaining 30 µl of FF samples were deproteinized by the addition of 260 µl of methanol, vortexed and centrifuged at 13400 g for 30 minutes. The supernatant was collected and the solvent evaporated. The obtained solid was subsequently dissolved in 540 µl of phosphate buffer with the addition of 60 µl of deuterated water with TMSP standard and 1D NOESY proton spectra were recorded on a Bruker Avance spectrometer with a 600 MHz magnet and a Broadband Inverse (BBI) probe, averaging 64 scans.
The obtained ATR and NMR spectra were uploaded to MATLAB (ver. R2017b, MathWorks), transformed into data matrices and class vectors were created, based on the patients' fertility. The data was then analysed by principal component analysis (PCA) and partial least squares-discriminant analysis (PLS-DA) methods, utilising the PLS_Toolbox (ver. 6.2, Eigenvector) software in the MATLAB environment.
Female infertility
FT-IR spectroscopy
NMR spectroscopy
Results:
For both ATR and NMR spectra, no meaningful data differentiation is observed in the PCA score plots, possibly due to being an unsupervised chemometric method and thus unable to detect relevant changes in complicated systems such as biological samples.
On the other hand, PLS-DA plots show clustering based on class for both sets of spectra, suggesting that there are detectable differences between the composition of follicular fluid of healthy women and those affected by infertility. This is supported by the PLS-DA loading plots resembling the difference spectrum between means of both sample classes.
Due to the FT-IR data separation being less pronounced, second derivative spectra were calculated using MATLAB. This drastically improved class differentiation, with no overlap between the clusters, suggesting that certain important variables in the ATR spectra are covered up by stronger vibrational modes of other molecules in the sample.
successfully used to discriminate between the two classes of samples, with potential to be utilised in routine infertility diagnostics.
that the composition of follicular fluid can provide valuable information as an infertility marker.
data points, suggesting the algorithm is too weak to distinguish between classes within complex systems.
methods, such as PLS-DA, is recommended.
M3/62
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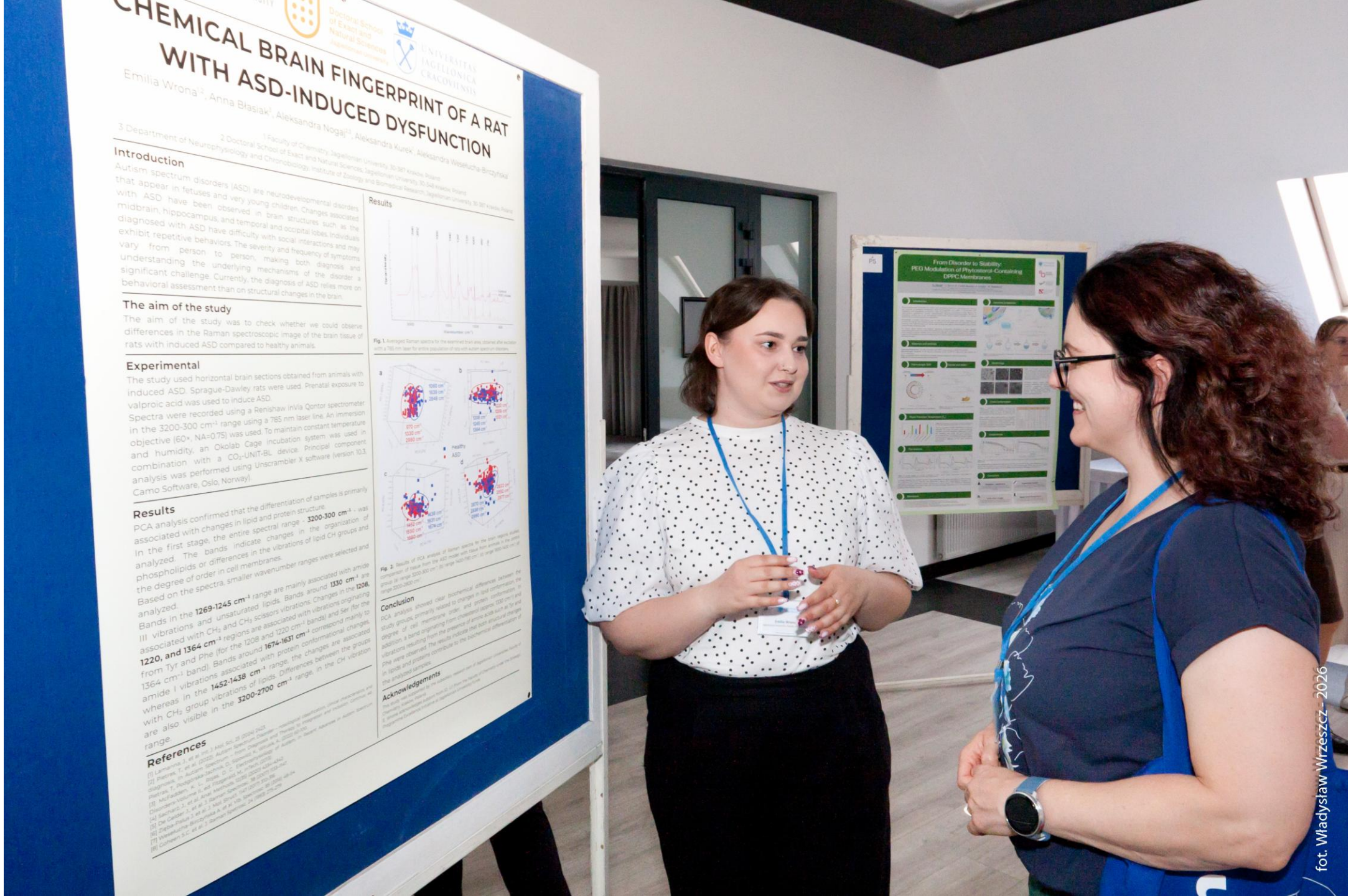
CHEMICAL BRAIN FINGERPRINT OF A RAT WITH ASD-INDUCED DYSFUNCTION
Introduction
The aim of the study
Experimental
Results
Conclusion
Acknowledgements
References
From Disorder to Stability: PEG Modulation of Phytosterol-Containing DPPC Membranes
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P#2
Association of menthol
Kewin Żmigrodzki, Kazimierz
University of Wrocław, Faculty of Chemistry, F. Joliot-Curie 14, Wrocław, 50-383, Poland
334224@uwr.edu.pl
Introduction
Methods
Experiment of non-linear dielectric measurements
Experiment of linear dielectric measurements
XRD Experiment
menthol/p-xylene
menthol/1,4-dioxane
Results
Discussion and conclusions
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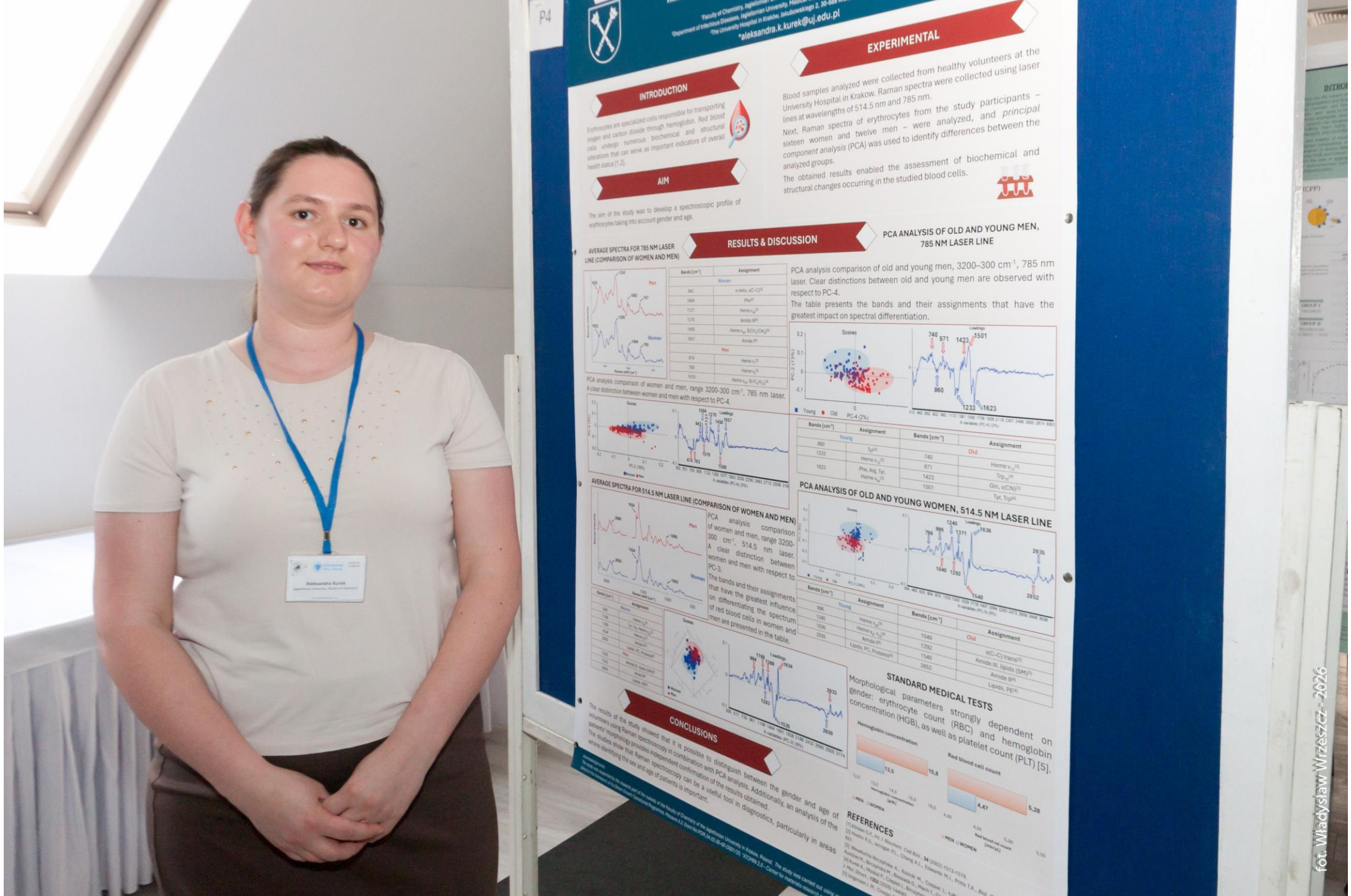
P4
INTRODUCTION
AIM
EXPERIMENTAL
RESULTS & DISCUSSION
CONCLUSIONS
STANDARD MEDICAL TESTS
REFERENCES
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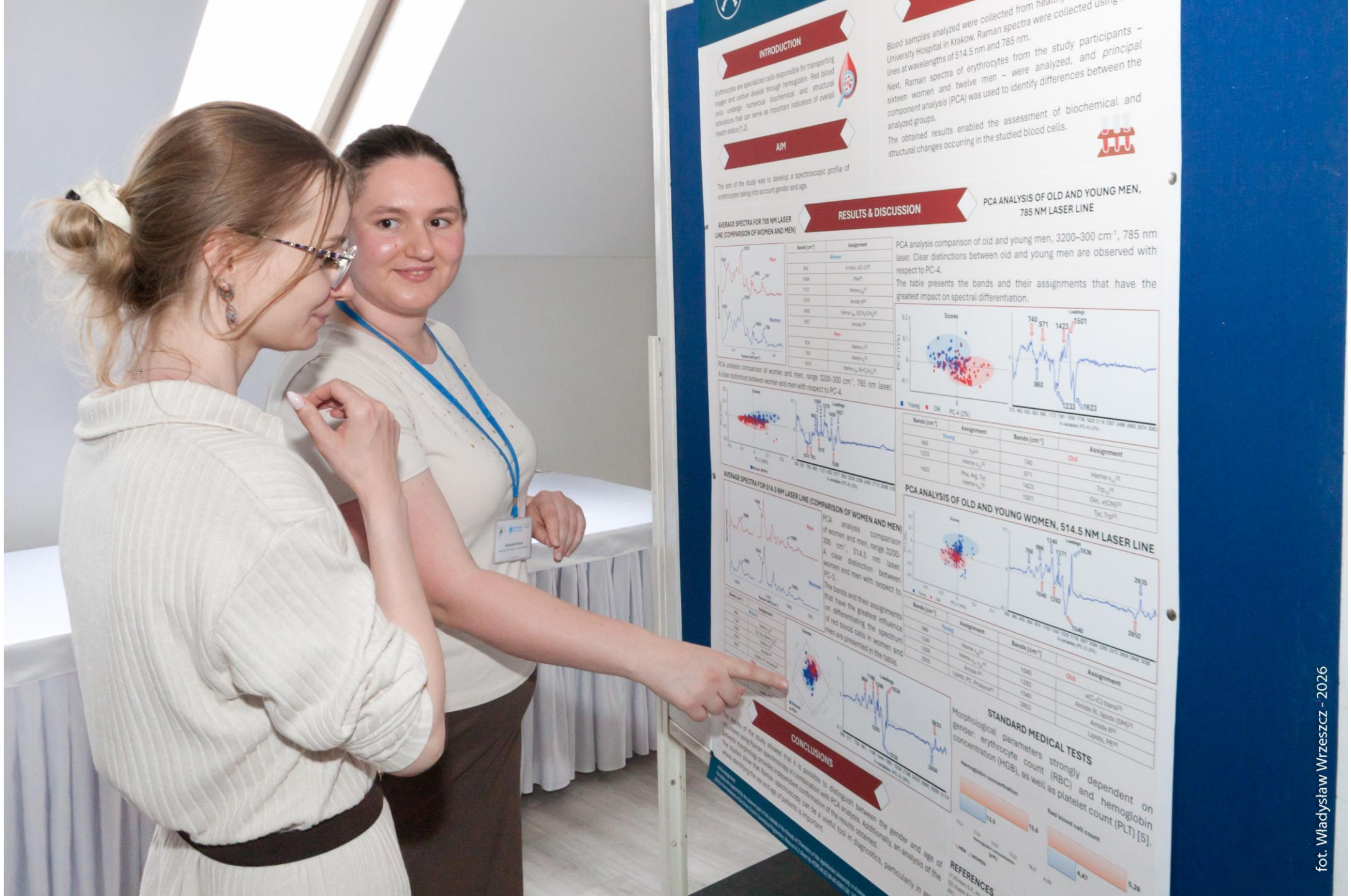

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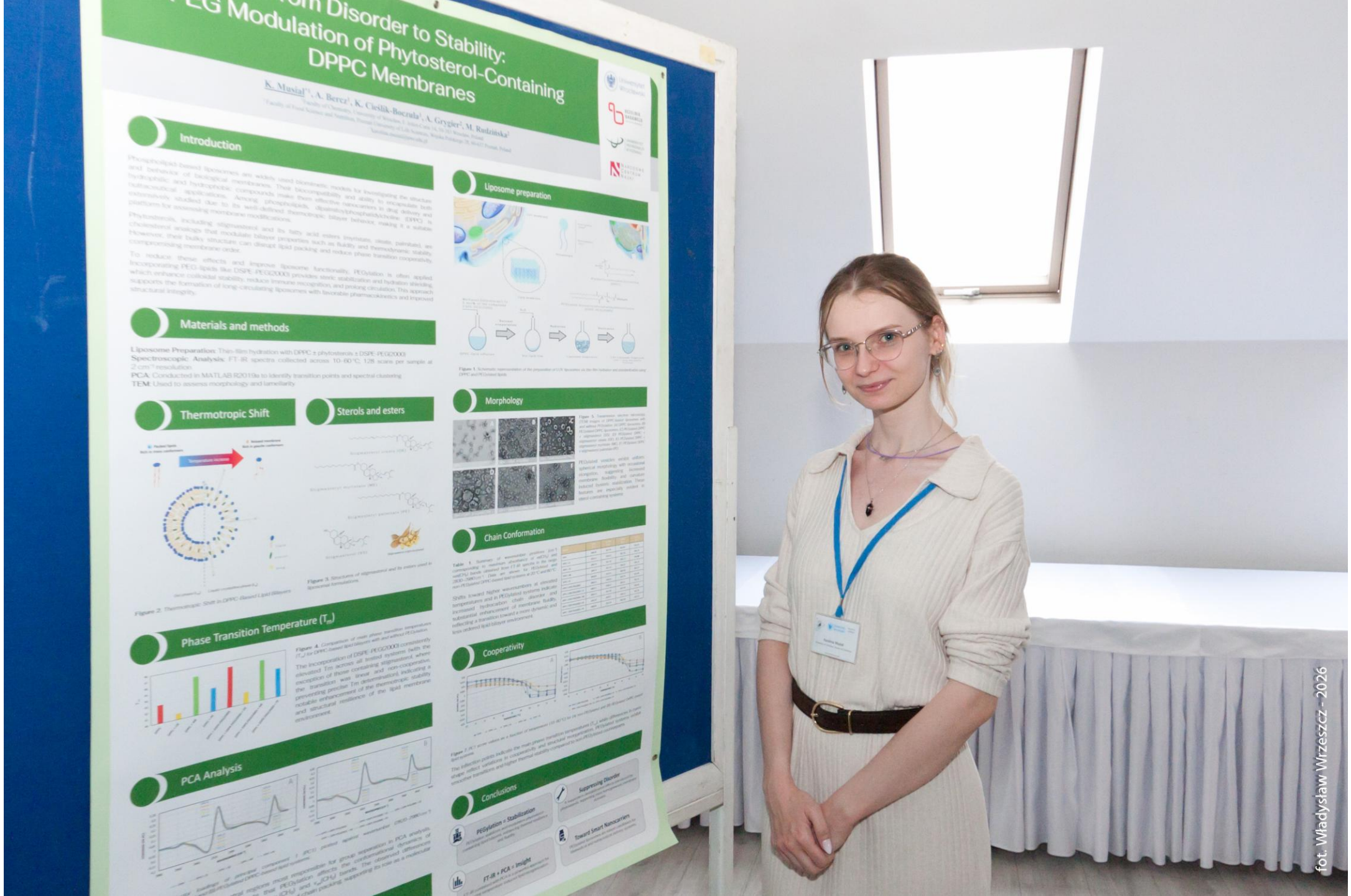
Order to Stability:
PEG Modulation of Phytosterol-Containing
DPPC Membranes
Introduction
Materials and methods
Liposome preparation
Thermotropic Shift
Sterols and esters
Morphology
Phase Transition Temperature (Tm)
Chain Conformation
Cooperativity
PCA Analysis
Conclusions
PEGylation = Stabilization
Suppressing Disorder
Toward Smart Nanocarriers
FT-IR + PCA = Insight
fot. Władysław Wrzeszcz – 2026

fot. Władysław Wrzeszcz - 2026

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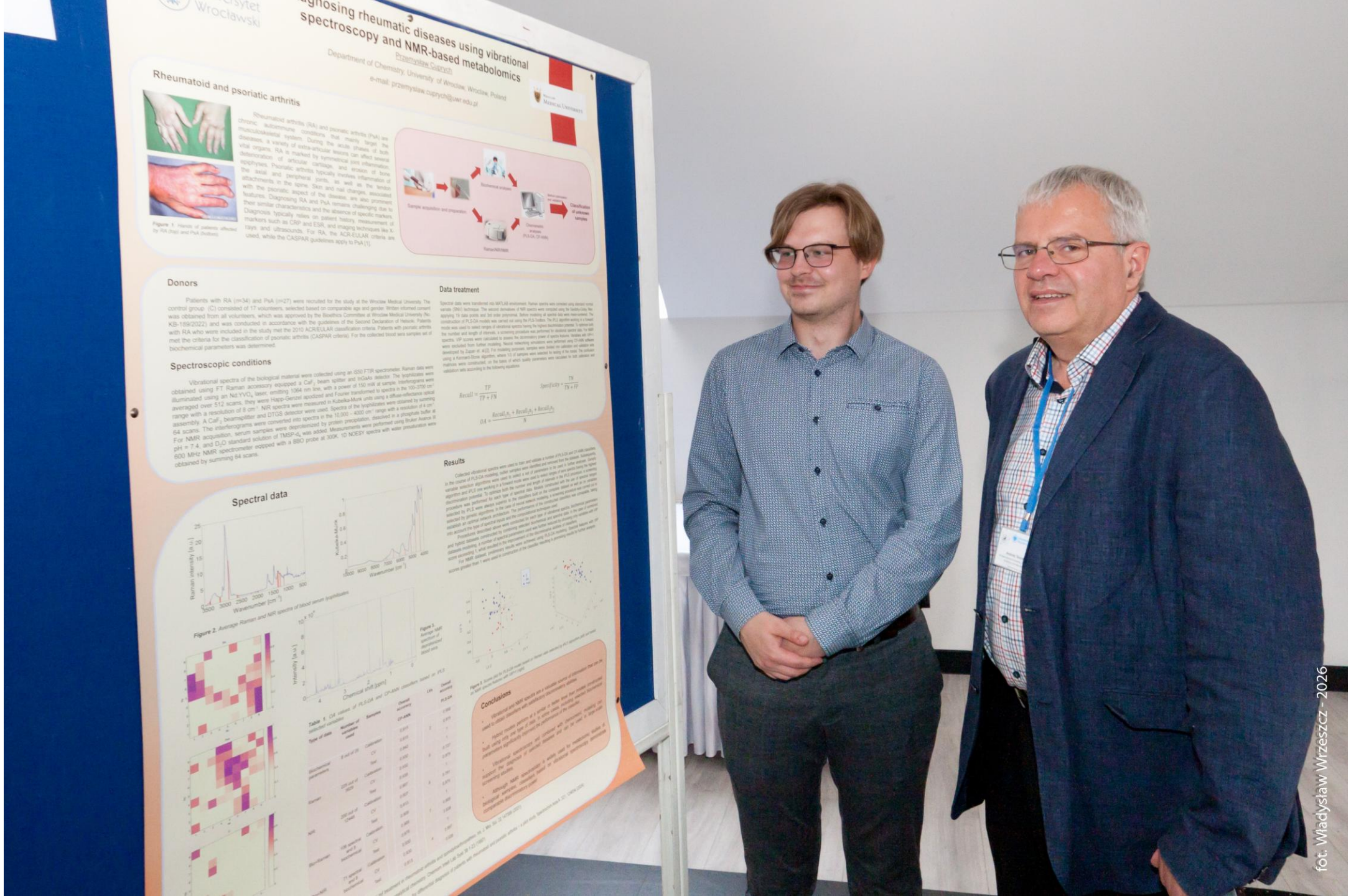
Diagnosing rheumatic diseases using vibrational spectroscopy and NMR-based metabolomics
Przemysław Cuprych
Department of Chemistry, University of Wrocław, Wrocław, Poland
e-mail: przemyslaw.cuprych@uwr.edu.pl
Rheumatoid and psoriatic arthritis
Donors
Spectroscopic conditions
Data treatment
Spectral data
Results
Conclusions
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Conference deliberations

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Diagnosing rheumatic diseases using vibrational spectroscopy and NMR-based metabolomics
P1
P3
P5
From Disorder to Stability:
PEG Modulation of Phytosterol-Containing DPPC Membranes
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The next European Meeting on Physical Organic Chemistry will be held in June 2027.

We warmly invite you to participate and look forward to welcoming you.