ML4NGP

MACHINE LEARNING FOR NON GLOBULAR PROTEINS

4TH MEETING on MACHINE LEARNING AND NON-GLOBULAR PROTEINS

19 – 22 May 2026

Targowa Creativity Centre, Warsaw, Poland

cost
EUROPEAN COOPERATION
IN SCIENCE & TECHNOLOGY

Funded by
the European Union

4TH MEETING ON MACHINE LEARNING AND NON-GLOBULAR PROTEINS

19 – 22 May 2026, Warsaw, POLAND

Welcome message

On behalf of the COST Action CA21160 *Non-globular proteins in the era of Machine Learning* (ML4NGP) and *the Institute of Biochemistry and Biophysics, Polish Academy of Sciences*, we are thrilled to welcome you to Warsaw for the 4TH ML4NGP Meeting.

As the last major gathering of our Action, this meeting is of exceptional importance to all of us who have contributed to the growth, energy, and scientific excellence of ML4NGP over the past years. It is a moment to celebrate our achievements, strengthen collaborations, and reflect on the impact our network has had on the research community.

This conference will once again bring together experts, young researchers, and innovators working at the intersection of Non-Globular Proteins (NGPs) and Machine Learning. Participants will have the opportunity to explore and discuss the latest developments in cutting-edge bioinformatic tools and specialised databases, research on repeats, intrinsically disordered regions, and low-complexity regions, and studies of proteins prone to aggregation or phase separation.

Whether you have been part of ML4NGP from the beginning or joined along the way, this meeting offers an exceptional platform to present your work, engage in thought-provoking discussions, and strengthen scientific connections that hopefully will continue long after the Action.

We warmly invite you to Warsaw to commemorate this milestone and to help shape the future directions of our community.

Organizing Committee

Marcin Grynberg, Katarzyna Jagiełło-Wilgat and Dorota Mężyńska from the Institute of Biochemistry and Biophysics, Polish Academy of Sciences, Warsaw, Poland

Core Group of ML4NGP COST Action

Keynote speakers

Prof. Rohit Pappu (Washington Univ. in St. Louis, USA)

Prof. Ben Schuler (University of Zurich, Switzerland)

Prof. Andrea Sinz (University of Halle-Wittenberg, Germany)

Prof. Tuomas Knowles (University of Cambridge, UK)

Registration

The registration desk will be open on Tuesday morning, May 19th, from 8:00 to 9:00.

Name Badges

Participants must wear their name badges at the venue and during social events, lunches, and dinners.

Internet access

Wireless Internet is available for free.

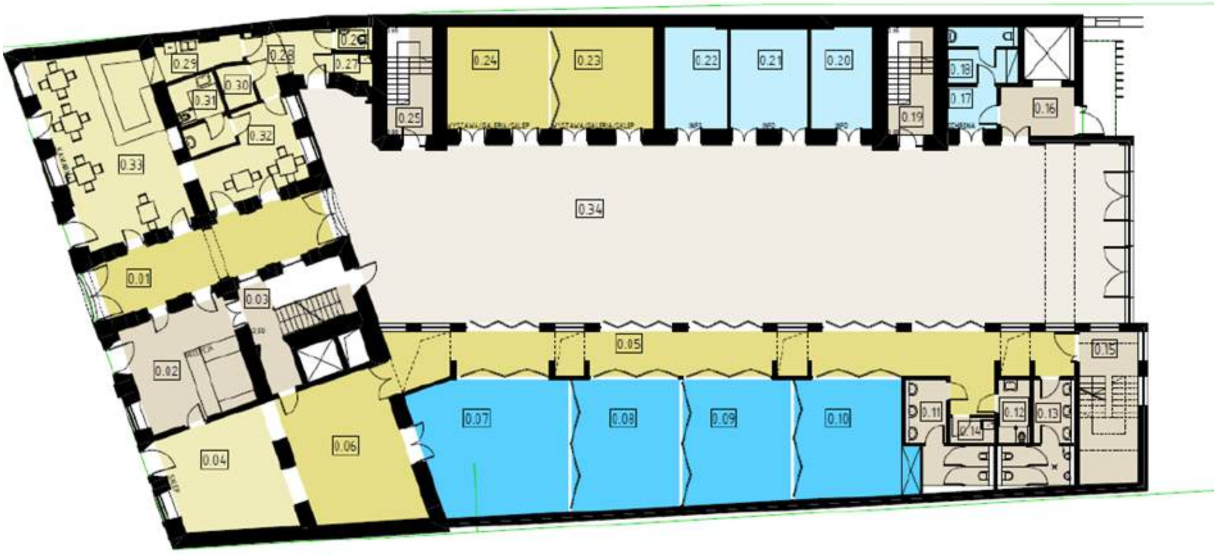
Venue rooms

Lectures will be held in the Różyc Room (0.07-0.10).

The poster presentations will be set up in the Main Hall (0.34).

Coffee breaks and lunches will also be provided in the Main Hall (0.34).

Main entrance and registration room: 0.02.



Location of the Conference Room (Różyc 0.07-0.10), poster sessions and coffee breaks (Main Hall 0.34).

Presentation guidelines

Poster guidelines

Posters should be up to **A0 size** – 118.9 cm x 84.1 cm (length x width). Poster numbers will be communicated to authors at the Registration Desk and can be found in the latter chapter of this booklet.

Poster presenters are requested to set up their posters in the designated area before the poster sessions. Poster presenters are encouraged to hang their posters on Tuesday, 19th May and remove them on Friday, 23rd May, during morning coffee break. Presenters are expected to be available near their posters during the assigned session. More information will be provided near the event.

Flash Poster Presentation

Selected poster abstracts should be presented as a slide presentation (5 min). Speakers are required to have their presentation ready on a USB key and contact technical staff during the coffee break before their session.

Oral presentation

Speakers are required to have their presentations ready on a USB key. Your slides should be either in .pdf, .ppt or .pptx format.

Speakers using their laptops are kindly asked to approach technical staff to clarify the technical prerequisites and coordinate the processes involved.

Presentation time

Since the meeting program is fully packed, we ask all presenters to keep to the time indicated for each presentation:

Keynote speaker talks - speaking time 35 min plus 5 min discussion

Invited talks - speaking time 25 min plus 5 min discussion

Selected talks - speaking time 12 min plus 3 min discussion

Flash presentations - speaking time 5 min

Social event and dinner

Welcome Reception - Tuesday, 19 May 2026 | 17:00

The Welcome Reception will be held at Targowa Creativity Centre Main Hall. All the participants are invited to have drinks and snacks.

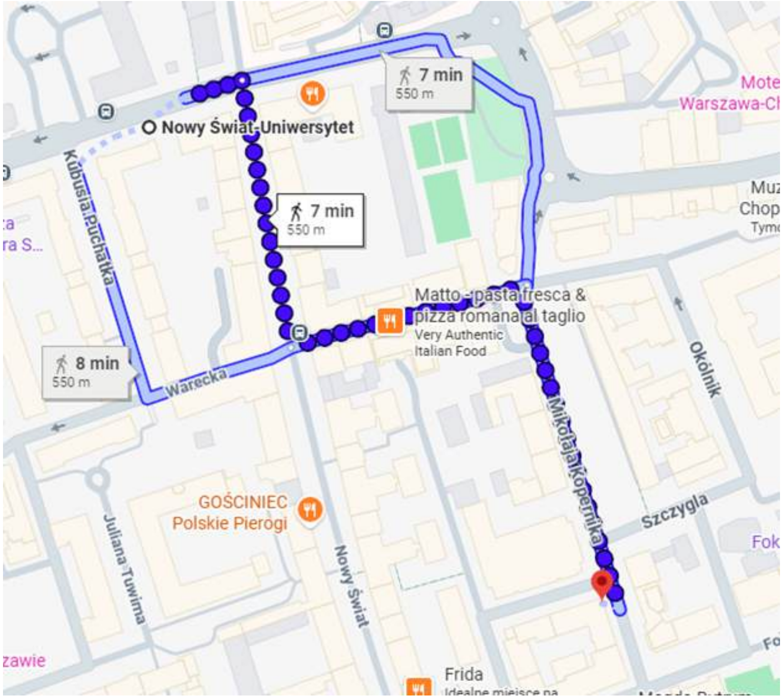
Social Dinner - Thursday, 21 May 2026 | 19:00 - 23:00 (arrival from 18:30)

The social dinner will be held on Thursday, May 21, 2026, at the Kameralna Restaurant (www.kameralnarestauracja.pl): https://maps.app.goo.gl/2oD3VJJVvrbYoAh7A?g_st=am

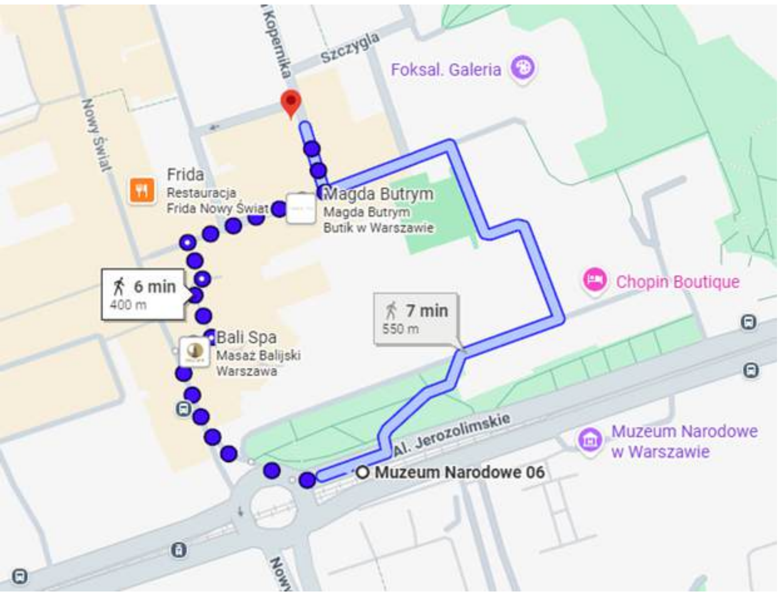
Kopernika Street 3

It is within walking distance from:

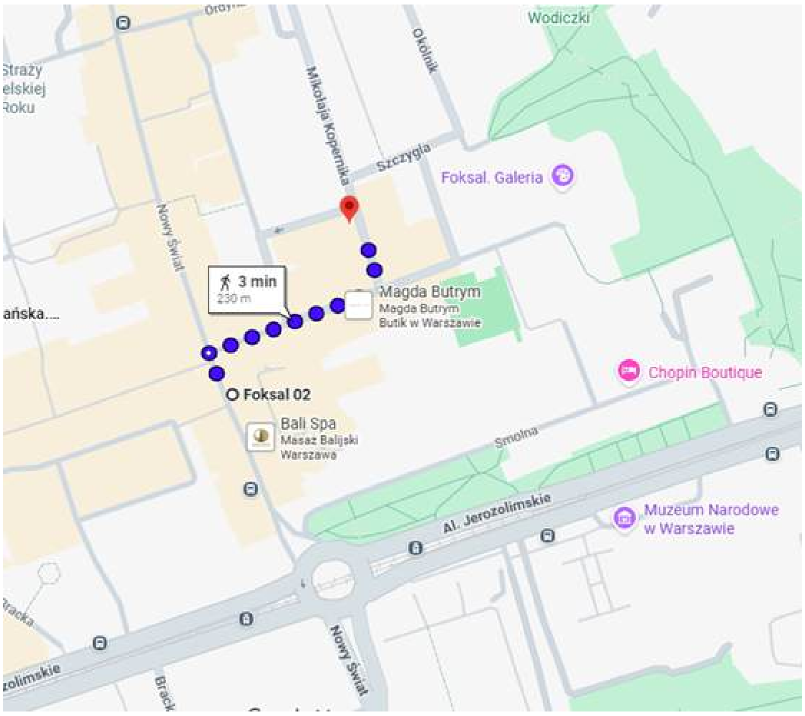
- Nowy Świat-Uniwersytet Metro Station (10 min)



- Muzeum Narodowe tram stop (8 min)



- Foksal bus stop (5 min)



Program

Monday, 18 May 2025

17:00 - 18:30 Core Group Meeting (closed session to the public)

Tuesday, 19 May 2026

8:00 – 9:00 Registration (room 0.02)

Różyc Conference Room (0.07-0.10)

9:00 – 09:15 **Opening Session**

Alexander Monzon

» Keynote Talk

9:15 – 9:55 **Phase transitions of RNA binding NGPs**

Rohit Pappu

» Invited Talk

9:55 – 10:25 **Beyond static structures: how protein language models help understanding protein flexibility**

Michael Heinzinger

» Selected Talk

10:25 – 10:40 **Generative design of intrinsically disordered proteins based on conditioned protein language models**

Juan Cortes

10:40 – 11:10 **Coffee Break**

» Invited Talk

11:10 – 11:40 **Peptide dynamics inside condensates on different scales**

Michael Feig

» Selected Talks

11:40 – 11:55 **Variant Effect Predictors in Intrinsically Disordered Regions are Systematically Biased**

Zsuzsana Dosztanyi

11:55 – 12:10 **Disordered and not so disordered proteins in bacterial biofilms**

Dirk Linke

12:10 – 12:25 **IDR-Mediated Nucleosome Engagement by the Pioneer Factor Sox2**

Sveinn Bjarnason

12:30 – 14:30 **Lunch Break** (Main Hall 0.34)

» Keynote Talk

14:30 – 15:10 **Probing the Rapid Interaction Dynamics of Charged Disordered Proteins**

Ben Schuler

» Selected Talks

15:10 – 15:25 **Achieving predictive all-atom simulations of disordered proteins and their condensates**

Miloš Ivanović

15:25 – 15:40 **Intrinsically disordered regions in mycobacterial transcription**

Lukáš Žídek

15:40 – 15:55 **Switch from a fuzzy to an ordered binding mode in the disordered regulator HigA2 mediates a ratio-sensing autoregulatory gene circuit**

San Hadži

16:00 – 17:00 **Flash poster presentations**

17:00 - 19:00 **Welcome reception** (Main Hall 0.34)

Wednesday, 20 May 2026

Różyc Conference Room (0.07-0.10)

» Keynote lecture

09:00 – 9:40 **Characterization of Intrinsically Disordered Proteins by Cross-Linking Mass Spectrometry**

Andrea Sinz

» Invited Talk

9:40 – 10:10 **Intrinsically Disordered Proteins Shape Organ-Specific Aging Trajectories**

Michal Sharon

» Selected Talk

10:10 – 10:25 **Ion mobility mass spectrometry unveils global protein conformations in response to conditions that promote and reverse protein phase separation**

Rebecca Beveridge

10:25 – 11:00 **Coffee Break**

» Keynote lecture

11:00 – 11:40 **Biophysical insights into IDP phase behaviour**

Tuomas Knowles

» Invited Talk

11:40 – 12:10 **Intrinsic disorder and fibril formation by the Henipavirus W proteins: molecular grammar and functional impact**

Sonia Longhi

» Selected Talk

12:10 – 12:25 **Structure-function studies of iron mineralization in extreme IDP confinement**

Raz Zarivach

12:30 – 14:00 **Lunch Break** (Main Hall 0.34)

14:00 – 16:00 **Round Table “Beyond the ML4NGP Action: Sustaining Collaboration, Open Science, and AI Responsibility in Non-Globular Protein Research”**

Salvador Ventura, Sonia Longhi, Miguel Andrade, Hamidreza Ghafouri, Zsuzsana Dosztanyi, Alexander Monzon, Silvio Tosatto (moderators: Zuzana Bednarikova, Rita Vilaça)

16:00 – 16:30 **Coffee Break**

16:30 – 18:00 **Poster Session I (odd numbers)**

19:00 Warsaw historic city centre tour (optional, based on registration)

Thursday, 21 May 2026

Różyc Conference Room (0.07-0.10)

» Invited Talks

09:00 – 9:30 **Molecular Models of Brain-Derived α-Synuclein Fibrils Reveal a Fuzzy-Coat-Mediated Mechanism for Selective Peptide Binding**

Salvador Ventura

9:30 – 10:00 **Chaperone-mediated regulation of tau phase separation**

Cláudio M. Gomes

10:00 – 10:30 **Beta-Arches as a Key Element in Improving Structure-Based and Machine-Learning Predictors of Amyloid Formation**

Andrey Kajava

10:30 – 11:10 **Coffee Break**

» Selected Talks

11:10 – 11:25 **Amyloid Proteins Through the Lens of AI Prediction Tools**

Malgorzata Kotulska

11:25 – 11:40 **Systematic mutational mapping reveals optimal amyloid formation for RIPK function**

Mariano Martín

11:40 – 11:55 **TMcluster: Nuanced clustering of protein structures using similarity matrices and dimensionality reduction**

Oriol Bárcenas

11:55 – 12:10 **Local frustration analysis reveals the energetic landscape of intrinsic disorder**

Franco Simonetti

12:10 - 12:25 **Exon-Informed Multiple Sequence Alignments for Enhanced Coevolution Signal Detection on Intrinsically Disordered Proteins**

Diego Javier Zea

12:30 – 14:30 **Lunch Break** (Main Hall 0.34)

» Invited Talks

14:30 – 15:00 **AI-based protein analysis from multimers to metagenomes**

Milot Mirdita

15:00 – 15:30 **Order within intrinsically disordered regions: function, structure and evolution**

Miguel Andrade

» Selected Talks

15:30 – 15:45 **Zero-Shot Prediction of Thermodynamic Properties of Proteins**

Gábor Erdős

15:45 – 16:00 **Machine Learned Coarse-Graining of Non-Globular Proteins**

Andrea Guljas

16:00 – 16:30 **Coffee break**

16:30 – 18:00 **Poster Session II (even numbers)**

19:00 - 22:00 **Social dinner**

Friday, 22 May 2026

Różyc Conference Room (0.07-0.10)

» Invited Talk

9:45 – 10:15 **Intrinsic disorder in the age of protein design**

Magnus Kjaergaard

» Selected Talk

10:15 – 10:30 **Generating conformational ensembles of multidomain proteins with flexible regions from AlphaFold models using AFflecto**

Mátyás Pajkos

10:30 – 11:00 **Coffee Break**

» Invited Talk

11:00 – 11:30 **Physics-Guided Diffusion Sampling for Conformational Variability**

Turkan Haliloglu

» Selected Talks

11:30 – 11:45 **MAPPIE: Map of Protein-Protein Interaction Embeddings for Functional Discovery**

Mert Cihan

11:45 – 12:00 **Large-scale proteomics and Deep learning for the generation of protein-protein interaction (PPI) maps at atomic resolution**

Jinmei Gao

12:00 – 12:15 **WormLink: A Tool for Engineering Synthetic Spacer Regions**

Laura Gherman

12:15 – 12:30 **Closing Remarks**

12:30 – 14:00 **Lunch Break** (Main Hall 0.34)

List of flash presentations:

F01 Nevena Ćirić: Hierarchical Deep Learning for Tandem Repeat Proteins Classification

F02 Julie Daniel: Exploring Binding Signals in Intrinsically Disordered Regions Through AlphaFold Embeddings

F03 Justas Dapkūnas: Homology-based analysis of protein structures and sequences with GTalign-web, COMER and PPI3D web servers

F04 Stanisław Dunin-Horkawicz: Detecting Non-Canonical Coiled-Coil Domains

F05 Aleksandra Gruca: LCRPlatform Update: Similarity-Based Annotation Transfer and Extended Functional Analysis of Low-Complexity Regions in Proteins

F06 Pavel Kadeřávek: Changes in the Dynamics of Microtubule-Associated Protein MAP2c upon Binding to the Regulatory Subunit of cAMP-Dependent Protein Kinase

F07 D. Kreil: Characteristic Positional Distributions of Functional Classes of Protein Regions with Compositional Bias, Structural Disorder, and Low Complexity

F08 Mahta Mehdiabadi: Modeling intrinsically disordered regions from AlphaFold2 to AlphaFold3

F09 Rafayel Petrosyan: A comparison of de novo designed amyloids with naturally occurring ones

F10 Milan Senćanski: Sequence-Based Discovery of Modulators for Disordered Proteins

F11 Darius Šulskis: The LLPS–Amyloid landscape of S100A and 14-3-3 proteins families

F12 Filippo Turchi: High-Resolution NMR Characterization of the Molecular Interplay between α-Synuclein, Fasudil, and Calcium Ions

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P01 Hanan Abdul Kareem: Prediction of Antimicrobial Peptide–Amyloid-β Interactions Using Transformer Language Models and Graph Attention Networks

P03 Maria Cristina Aspromonte: Interpreting missense variation in intrinsically disordered proteins

P05 Jan Beránek: Monte Carlo simulations of miniprotein folding sampled with an autoencoder

P07 Ahmed Abdeldjalil Bouziane: Substitution Matrix for Improved Analysis of Low Complexity Protein Sequences

P09 Ondrej Cehlar: Disordered oligomers formed by truncated tau proteins

P11 Alisa Davtyan: AmyloDeep: pLM-based ensemble model for predicting amyloid propensity from the amino acid sequence

P13 Radovan Dvorsky: From SPuRs to Retrieval and Classification of Protein Fragments Defined by Sequence–Structure–Interaction Constraints

P15 Vaclav Hanzl: Mapping conformation landscapes hidden in ESMFold protein language models

P17 Valentín Iglesias: A4D Antibody Aggregation Database (A4D-ABDB): identifying and optimizing aggregation propensity for therapeutic antibodies.

P19 Filip Kapral: Atlas of amino acid roles in human proteins

P21 Cajsa Malm: NMR-Validated Molecular Dynamics Reveals Phosphate-Induced Ordering in Recombinant Spider Silk Protein

P23 Katarína Martonová: Experimental and AlphaFold modelling of short regions in the disordered tau fragment dGAE engaged in complexes

P25 Pablo Mier: Amino acid homorepeats in tape measure proteins correlate with bacteriophage tail length

P27 Segev Naveh-Tassa: Multivalent Tau–Microtubule Interactions as a Case Study in Non-Globular Protein Function

P29 Kliment Olechnovic: Tessellation-based comparison of conformations, interfaces, and ensembles of non-globular proteins

P31 Max Pawlyta: Towards a Structural Understanding of the Intrinsically Disordered Actin-Binding Protein Synaptopodin

P33 Santiago Rodriguez: SAXS–Guided Modeling of the Aryl Hydrocarbon Receptor–Hsp90 Complex and Its Assembly with Importins

P35 Mariia Rutkowska: AmyloGraph Ab-DB: A Resource for Amyloid–Antibody Interactions

P37 Rostislav Skrabana: Extracting disorder information from ordered structures deposed in PDB

P39 Alessia Strappazzon: Differential Regulation of p27 Stability by VHL Isoforms and the Cancer-Associated p27E40K Mutation

P41 Guglielmo Tedeschi: CVFormer: Data-Driven Collective Variables via Transformer Autoencoders

P43 Soma Varga: On the menu today: NMR studies of the intrinsically disordered actin-binding region of Drebrin

P45 Nenad Vilendečić: Structural Roles of IDPs in Dynamic PPI Networks

P47 Esra Yuca Yilmaz: From Repeated Peptide Motifs to Functional Biomaterials: Recombinant Elastin-Like Polypeptides as Tunable Protein Polymers

P49 Julia Ciezsko: Analysis of bacterial amyloids potentially involved in neurodegeneration using updated AmyLoad database

Poster session II

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F12 Filippo Turchi: High-Resolution NMR Characterization of the Molecular Interplay between α-Synuclein, Fasudil, and Calcium Ions

P02 Matteo Arnaudi: An Integrative structure-based approach to link diseases associated mutations to pathogenicity

P04 Zuzana Bednarikova: Oligomeric-State-Dependent Inhibition of Aβ40 Aggregation by the 14-3-3ζ proteins

P06 Nerea Blanco: Homorepeat Overlap in Orthologs: Evolutionary Insights into Swappable and Non-Swappable PolyX Regions

P08 Marianna Bussolino: Recombinant expression and purification of pVHL isoforms in E. coli for in vitro screening of small molecules

P10 Jarosław Chilimoniuk: Mapping the landscape of antidiabetic peptides: toward a curated literature-derived database

P12 Dragana Dudic: Disorder-based profiling of plant stress proteins

P14 Hamidreza Ghafouri: Experimentally Refined Conformational Ensembles of Intrinsically Disordered Proteins from SAXS Data

P16 Richárd Hornyák: Benchmarking Computational Methods to Characterize the Conformational Ensembles of Intrinsically Disordered Proteins

P18 Kamil Kamiński: Detecting non-canonical coiled coils beyond state-of-the-art methods

P20 Arnau Francesca Llaberia: Energy Landscape Consequences of Disulfide Bonds in Proteins

P22 Simona Manasra: AmyloComp-3D: A Structure-Based Predictor of Amyloid Co-Aggregation

P24 Ana Melo: Impact of Anionic Aggregation Inducers on Disease-Associated Tau Mutants

P26 Kamile Mikalauskaite: Characterization of Alpha-synuclein Fibrils with Highly Divergent Thioflavin-T Binding Properties

P28 Stefana Njemoga: N-terminal truncation of tau dGAE (297–391) highlights the importance of residues 321–325 in early fibril formation

P30 Kristinn Ragnar Óskarsson: Long-range cross talk between intrinsically disordered regions modulates FOXA1 interactions with DNA

P32 Shira Peer: Disordered Tails of Myc:Max Regulate DNA-Binding Kinetics and Specificity via Transient Competition

P34 Magnús Rúnarsson: Using Single-Molecule FRET to Decipher the Effects of Oncogenic Mutations on the Pioneer Factor FOXA1

P36 Tomáš Sádecký: Ligand docking into the truncated tau dimers as targets for design of small molecular therapeutics

P38 Kristina Stevanović: Long-Range Interaction–Driven Identification of Carbonic Anhydrase Inhibitors as Direct Tau Binders

P40 Mattia Utichi: Ensemble structural analysis reveals how flanking regions modulate LIR motifs in intrinsically disordered autophagy receptors

P42 Marija Vidovic: Inhibitory Potential of LEA Proteins from Ramonda serbica on the Aggregation of A53T α-Synuclein

P44 Damian Michal Wilary: Transparent AI-Assisted Discovery of Antibody–Amyloid Interaction Studies from Abstract-Level Evidence

P46 Mantas Ziaunys: Cryo-EM Analysis of Alpha-Synuclein Fibril Structures Formed under Different Temperature Conditions

P48 Diego Javier Zea: AlphaFold 3 Modeling of the KfrA–KfrB–KfrC R751 System Suggests a Shared KfrB Interface and Ion-Sensitive KfrA Stability

P50 Kemal Demirtaş: IDP-Specific Coevolution and Dynamics-Aware Modeling Enable Prediction of Allosterically Competent Binding Sites

Event Venue

The Meeting will take place at the **Targowa Creativity Centre** (cktargowa.pl).

Address: Targowa 56, 03-733 Warsaw, Poland

Google map link: https://maps.app.goo.gl/4a4pTene2MWd9sP19?g_st=am

Timetables, connections within the City of Warsaw: https://www.wtp.waw.pl/en/

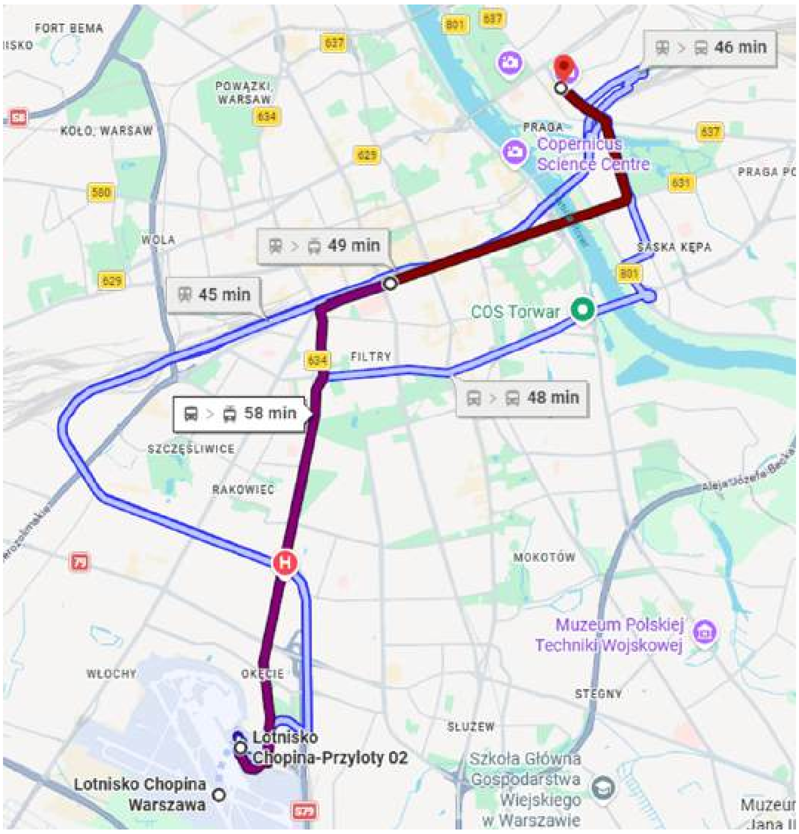
Arriving at the Targowa Creativity Centre from the Warsaw Chopin Airport

The Chopin Airport (WAW) is within the city limits: take the 175 bus to Dworzec Centralny (Central Railway Station) stop. Switch to the 25 tram (dir. Praga/Annopol). Leave the tram at the Ząbkowska stop: The Targowa Creativity Centre is on the other side of Targowa Street.

In order to reach the Targowa Creativity Centre, purchase the 75-min., 4,40 PLN ticket.

Other public transportation options from the Chopin Airport:

https://www.wtp.waw.pl/en/public-transport-step-by-step/airports-transport/



Arriving at the Targowa Creativity Centre from the Warsaw Modlin Airport:

Warsaw Modlin Airport (WMI) is located 40 km north of the centre of Warsaw.

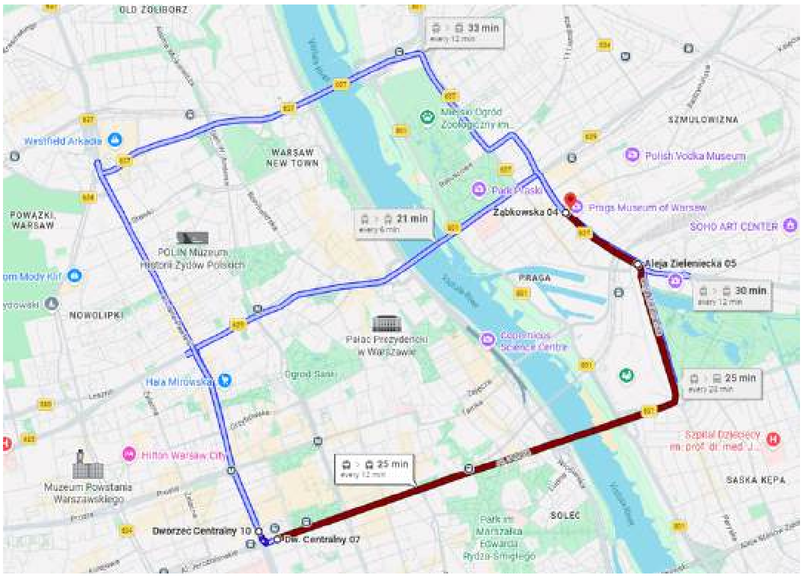
Warsaw Public Transport **does not serve Modlin Airport**. Access is provided by Mazovia Railways trains (to Modlin station) or direct shuttle buses.

All information on how to get to and from Modlin is available on the Warsaw Modlin Airport website: en.modlinairport.pl

Arriving at the Targowa Creativity Centre from the Central Railway Station:

Take the 25 tram (dir. Praga/Annopol). Leave the tram at the Ząbkowska stop: The Targowa Creativity Centre is on the other side of Targowa Street.

In order to reach the Targowa Creativity Centre, purchase the 20-min., 3,40 PLN ticket.



Other railway stations in Warsaw: https://www.wtp.waw.pl/en/bus-and-railway-stations/

Where to buy tickets:

- Ticket machines located in most transport points (cash or payment card).
- Ticket machines in vehicles (payment cards).

Ticket machines operate in Polish, English, German, Russian, and Ukrainian.

- Several mobile apps: https://www.wtp.waw.pl/en/where-to-buy-a-ticket/ticket-by-mobile/

Note:

The City of Warsaw has granted free public transport tickets to all conference Participants.

Tickets will be issued during on-site registration at the Targowa Creativity Centre. Each Participant will receive four 24-hour tickets (one for each day of the conference; tickets should be validated every morning), therefore Participants are only required to arrange their transportation to the conference location upon arrival.

Organization

ML4NGP MACHINE LEARNING FOR NON-GLOBULAR PROTEINS

cost EUROPEAN COOPERATION IN SCIENCE & TECHNOLOGY

Funded by the European Union

This event is part of the activities of the COST Action ML4NGP, CA21160, supported by COST (European Cooperation in Science and Technology).

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Ministry of Science and Higher Education Republic of Poland

WEKTORY NAUKI

This event is part of the activities of the COST Action ML4NGP, CA21160, supported by COST (European Cooperation in Science and Technology).