NEWSLETTER

JUNE 2024

ML4NGP COST ACTION | ED. 2

By Rita Vilaça | Science Communication Coordinator

2ND ML4NGP MEETING

THESSALONIKI, GREECE | 14-17 MAY 2024

The vibrant city of Thessaloniki, Greece, was the stage for the organization of the 2nd ML4NGP Meeting on Machine Learning and Non-globular Proteins. This landmark event was co-organized with MSCA-RISE project REFRACT.

The conference featured a top-level scientific program, with 4 keynotes, 5 five selected talks and 28 short talks. Additionally, 64 posters were presented, with 11 chosen for flash poster presentations. The diverse range of topics covered the interdisciplinary and innovative research in the field of machine learning (ML) for non-globular proteins (NGPs).



OUR KEYNOTE SPEAKERS



The keynote talks highlighted the transformative potential of new machine learning algorithms for understanding protein structures, sequences, and functions. They also addressed the challenges and innovative approaches in drug discovery for intrinsically disordered proteins (IDPs) associated with amyloid diseases, and the importance of accurate protein structure prediction through the Critical Assessment of Structure Prediction (CASP). The concept of the virtual proteome of life was revisited, as well as a comprehensive overview of the evolution of bioinformatics from proteins to IDPs, globular showcasing significant strides and a promising future in the field.

"The 2nd Machine Learning and Non-Globular Protein (ML4NGP) Meeting, which drew nearly 130 scientists from 34 countries, underscored the global importance and collaborative spirit of our research area. It was inspiring to see researchers from various fields and career stages come together in lively discussions to explore novel advancements in machine learning methods to study non-globular proteins. The meeting gathered various experts in the field, ranging from experimentalists to those developing computational methods. This multidisciplinary atmosphere positively contributed to interesting discussions about the next challenges in the field."

ALEXANDER MONZON & ZUZANA BEDNARIKOVA, ACTION CHAIRS



ML4NGP MEETING

The meeting set the stage to a global exchange of knowledge covering a wide range of topics, reflecting the dynamic and multifaceted nature of non-globular proteins research. Among them:



A vibrant atmosphere with amazing speakers at the 2nd ML4NGP Meeting, in Thessaloniki Greece.

The conference recognized the outstanding contributions of young researchers with four awards for the best posters:

"Exploration of the vibrational space of tandem repeat proteins" by Matias Chiappinelli "Exploring the Impact of Intrinsically Disorder Regions on RNA stability and microRNA Accessibility" by Mert Cihan

"Self-assembling protein-based nanoparticles for biomedical and biotechnological applications" by Marc Fornt Suñé

"Effects of the ionic strength on functional amyloid fibril formation" by Andrea Bartolomé-Nafría



What part of the meeting did you enjoy the most?

The possibility to disseminate my work in a short talk and the networking options to collaborate with other researchers.

The outstanding scientific program, along with the quality of the speakers and poster presentations.

Networking and reconnecting with researchers from past conferences.

WG meetings and discussions over lunches and coffee breaks.

Presentations of experimental results which were connected with ML approaches.

enjoyed presentations, particularly because they provided deep insights into the advancements and applications of machine learning for non-alobular proteins.

the

keynote

really

ML4NGP MEETING

During the conference, dedicated working group (WG) meetings actively engaged participants in shaping the future directions of the ML4NGP COST Action. These discussions facilitated collaboration and the exchange of ideas, advancing the next steps for each working group.



Working Group 1 meeting focused on practical issues related to the generation of reference datasets (one of the tasks of Working Group 1), so that they can be effectively used in the **development of computational tools for predicting structural features and dynamics** of disordered proteins. In addition, it was discussed strategies to improve the **understanding of the information provided by experimental data to computational scientists** in order to improve their interpretation of raw data.

The working group 2 discussed strategies to integrate **structural biology with ML-based approaches** for determination of non-globular structures. Researchers outlined critical research areas and goals for the next year, including developing ML-based approaches for predicting structural ensembles of IDPs and the **need for experimental data to benchmark these predictors**. They also discussed the **validation of non-globular protein ensembles** and the development of ML-based tools to predict NGP functions.

The working group 3 concentrated on discussion regarding NGP structural ensembles prediction challenge. It was suggested that it is necessary to carefully define the challenge problem, to generate reference datasets for unbiased assessment of ML predictors against experimental data and to determine the apropriate evaluation metrics. WG3 plans to continue to work on the keypoints of the discussion in the following period.



The working group 4 meeting aimed to advance the functional characterization of non-globular proteins. In particular, it is was discussed how future work should address the **development of computational tools for predicting the effect of mutations on NGPs structures** and link with function/dysfunction. Also, it was discussed how AlphaFold is not able to answer all the challenges for prediction of NGPs structures.

Within the WG5 activities, the participants were challenged to be a science communicator for one day. Working in diverse they groups, developed strategies to explain key nontopics like machine learning, globular proteins, and protein aggregation to various audiences, including young children, high school teachers, and funding agencies, contributing to help bridge the gap between ML4NGP and the public.



Participants at the 2nd ML4GP meeting engaging into science communication activities.

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ML4NGP MEETING

The ML4NGP meeting in Thessaloniki was a resounding success, uniting a diverse group of experimental and computational researchers to share their latest findings and forge new collaborations. The insights and innovations presented highlighted the pivotal role of machine learning in advancing our understanding of non-globular proteins, paving the way for future discoveries and therapeutic breakthroughs.



Group photo with the participants and speakers in front of ONOMA Hotel during the 2nd annual ML4NGP meeting, in Thessaloniki, Greece.

A special comment about the 2nd ML4NGP Meeting

"The ML4NGP 2024 meeting was an outstanding introduction to the world of protein disorder. I have rarely met such a passionate and focused academic community, and the impact and urgency of understanding protein disorder was made very clear through the compelling talks and student posters. I left the conference with a new perspective on how machine learning might play a role in this topic, and optimism that this strong community is poised to make breakthroughs in this space."

Joshua Pan | Google DeeMind

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