NEWSLETTER

NOVEMBER 2024

ML4NGP COST ACTION | ED. 3

By Rita Vilaça | Science Communication Coordinator

We're back with another edition of the ML4NGP newsletter, bringing you the latest news about our Action. This edition includes a consice overview of our events, as well as a selection of testimonials from our grantees. You can also found information on the planned activities for the next grant period. We invite you to take a look at what's new and exciting in the world of machine learning and non-globular proteins!

MAIN MEETING

The 2nd ML4NGP Meeting on Machine Learning and Non-globular Proteins took place in Thessaloniki, Greece, from 14 to 17 May. The scientific program featured four keynotes, five selected talks, 28 short talks, and 64 posters, of which 11 were highlighted as flash poster presentations. The meeting showcased innovative and interdisciplinary research at the intersection of machine learning and non-globular proteins.

READ MORE ❯

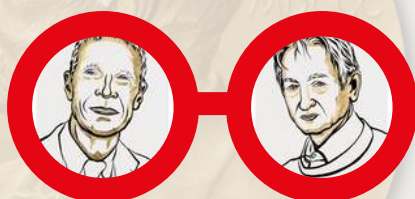## CELEBRATING NOBEL PRIZES

THE NOBEL PRIZE IN CHEMISTRY

David Baker   Demis Hassabis   John M. Jumper

THE NOBEL PRIZE IN PHYSICS

John J. Hopfield   Geoffrey E. Hinton

Laureates photos designed by Niklas Elmehed © Nobel Prize Outreach

The 2024 Nobel Prizes in Physics and Chemistry mark a significant milestone for the ML4NGP COST Action. This groundbreaking recognition of advancements in artificial neural networks by John Hopfield and Geoffrey Hinton, on computational protein design by David Baker and in AlphaFold by Demis Hassabis and John M. Jumper, directly aligns with our mission to revolutionize the study of non-globular proteins. Through the development of innovative machine learning tools, we aim to uncover the unique structural and functional properties of these fascinating proteins—advancing a vision shared by this year's laureates.
This achievement highlights the transformative potential of computational science in unraveling biological complexity.

A proud moment for our community and a bright future ahead!

SECOND YEAR IN REVIEW

TRAINING SCHOOL

The 2nd ML4NGP Training School was locally organized by Damien Devos in Carmona, Spain. During 4 intensive days, the participants and trainers explored the latest advancements on computational tools to study non-globular proteins. This Training School focused on the latest advances and current challenges for characterization of tandem repeat proteins, intrinsically disordered proteins, low complexity regions and protein aggregation, among other topics.

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Participants and trainers during the theoretical lectures and hands-on practical sessions at the 2nd ML4NGP Training School in Carmona, Spain.

WORKSHOP

The 3rd ML4NGP Workshop was held from 25 to 27 September, at the Instituto Superior Técnico, in Lisbon (Portugal). The workshop was attended by 31 participants from 14 countries. The workshop aimed to bring together leading experts in the field of single-molecule FRET to discuss the basis for establishing a FRET database. The workshop featured an exceptional program with 22 seminars

Group Photo with participants and speakers of 3rd ML4NGP Workshop.

about smFRET and simulations integrating FRET data. The talks covered intrinsically disordered proteins under functional and aggregation conditions, globular proteins and DNA-protein interactions, and also analysis models and accuracy/reproducibility in smFRET.

Participants attending the 3rd ML4NGP Workshop on single-molecule FRET for Non-globular proteins organized in Lisbon, Portugal.

The workshop was an opportunity to discuss the complexity and diversity of smFRET data and the deposition of fluorescence parameters. The possibility of future grant applications for the implementation of a smFRET database was also discussed. A working group was defined to set up the minimum information required for the integration of the FRET database, which will then be shared with the FRET community.

FULL PROGRAM ❯

SECOND YEAR IN REVIEW

EXPANDING HORIZONS WITH NSF

ML4NGP AT THE 6TH ACCELNET MEETING IN THE USA

Alexander Monzon, Action Chair of ML4NGP COST Action, was invited to participate in the prestigious AccelNet 6th Annual Meeting for Principal Investigators, held in Washington, DC. This event provided a unique opportunity to network with global research leaders and explore potential cross-border collaborations. NSF funded AccelNet program and COST Actions share a common goal to foster international partnerships and advance scientific research. This participation promises to open doors for new multidisciplinary projects and collaborations between Europe and the USA.

READ MORE ⊙

MOBILITY AND TRAINING

ML4NGP GO GLOBAL: SCIENTIFIC MISSIONS AND CONFERENCE GRANTS

8 STSMs
3 ITC-CG

South Korea

In the second grant period, three researchers from inclusiveness target countries were awarded with conference grants allowing them to share their research work at high level international conferences.

We also provided funding for eight short term scientific missions for mobility and training of researchers among different countries and institutions.

These funding opportunities are a great opportunity to support scientific research and foster collaboration among the Action's members and contribute for personal and institutional capacity-building.

FEEDBACK

I'd like to sincerely thank COST Action ML4NGP STSM and BiocomputingUP for giving me this amazing opportunity to work with the BiocomputingUP lab for two months. As a computer science PhD student, this experience was invaluable in expanding my understanding of protein aggregation through collaboration with experienced researchers in bioinformatics. It opened my eyes to the exciting possibilities of applying computer science techniques to protein-related predictions.

I have always enjoyed being an exchange researcher and collaborating with different groups, as it provides an excellent opportunity to gain knowledge and work efficiently in a new environment. Lastly, Padua is a beautiful city with great food, and I may have never thought of visiting it if not for this exchange opportunity.

DI MENG
Visiting Researcher at the University of Padova, Italy

SECOND YEAR IN REVIEW

FEEDBACK

ERDŐS GÁBOR

Attendee at 23rd European Conference on Computational Biology in Turku, Finland.

How did the ITC Conference Grant provide you with the opportunity to share your work on ECCB2024 in Turku?

The conference grant enabled me to travel and present at the ECCB conference in Turku, Finland. Given that ECCB is one of the largest computational biology conferences globally, it provided me with the opportunity to share my work with a broad audience. Without the grant, I wouldn't have been able to attend, making the ITC Conference Grant essential in allowing me to present my research to a wider community.

In what ways did your participation in the conference enhance the dissemination and visibility of your work within the international scientific community?

As one of the largest conferences in computational biology, the ECCB meeting offered an excellent platform to share my work. It provided an exceptional networking environment, not only with the general scientific audience but also with various scientific consortia and industry partners. I had the chance to reconnect with colleagues, exchange new ideas, pose intriguing questions, and plan future collaborations. Additionally, I met several new groups, with whom I am excited to explore potential future collaborations.

Did you receive any feedback or comments during the conference that could lead to potential future collaborations?

In that regard I was very fortunate. I was able to meet with some colleagues who I haven't seen in a long time, and had some great discussions about a specific project which we are planning to start early 2025.

HAMIDREZA GHAFOURI

Visiting Researcher at University of Copenhagen, Denmark.

How did the experience you gained at the University of Copenhagen contribute to advancing your PhD?

My Short-Term Scientific Mission (STSM) at the University of Copenhagen, specifically in Prof. Lindorff-Larsen's lab, had a significant impact on advancing my PhD research. As one of the world's leading groups in studying intrinsically disordered proteins (IDPs), the lab provided me with the opportunity to familiarize myself with cutting-edge tools and software packages developed for IDP research and simulations. Additionally, since our lab at the University of Padova maintains key databases on IDPs, such as DisProt and the Protein Ensemble Database (PED), the knowledge and skills I gained at the University of Copenhagen will enable me to contribute to enhancing these databases, which is a critical objective of my PhD.

Were you able to learn new techniques or gain access to resources that were not available at your home institution? Can you give some examples?

Yes, during my STSM, I had the opportunity to learn new techniques. One key example is the coarse-grained simulation of intrinsically disordered proteins (IDPs) using the recently developed method CALVADOS-3. This method, which was a highlight of my experience, allowed me to simulate the dynamics of disordered proteins with multiple domains. I also gained valuable experience in analyzing the resulting data, such as the compactness of the IDR ensembles of the DisProt database.

Can you share a specific example of how the work you performed will influence or improve your PhD project?

One specific example is the simulation of all intrinsically disordered regions (IDRs) from the DisProt database using the CALVADOS method. This allowed me to generate conformational ensembles for these regions, which will be published in the Protein Ensemble Database (PED). These ensembles will not only enrich the PED but also provide valuable insights into the global properties of IDRs, such as their degree of compaction. This information is crucial for studies on the relationship between ensemble structures and protein function, which is a key focus of my PhD research.

How do you think this experience has influenced your future research plans or career prospects?

I believe this STSM was an invaluable opportunity that has significantly influenced both my future research plans and career prospects. It exposed me to cutting-edge techniques and methodologies, such as the CALVADOS simulation method. This experience has not only expanded my technical skills but also sparked new ideas for my research on intrinsically disordered proteins (IDPs).Moreover, the opportunity to collaborate with renowned experts in the field has expanded my professional network. These connections could lead to future collaborations.

SECOND YEAR IN REVIEW

»» ML4NGP VIDEO TO CELEBRATE OUR 2ND ANNIVERSARY ««

Our ML4NGP YouTube channel is now live!
If you have any relevant content you'd like to contribute, such as webinars, open lectures, or informative videos, just reach out, and we'll be happy to feature them on our channel!

We are also very happy to share our brand-new video, which gives an insight into our mission, our network, and the many opportunities for collaboration, knowledge sharing, and funding! We believe this is a milestone as our Action continues to gorw with new members joining every month! Don't forget to like, comment and share!
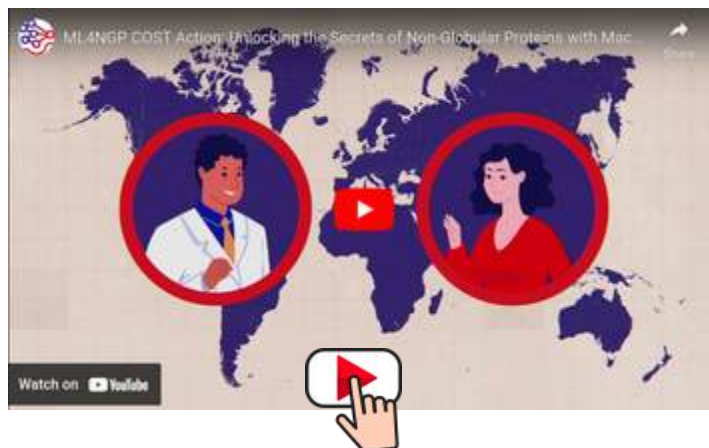
ML4NGP TALKS
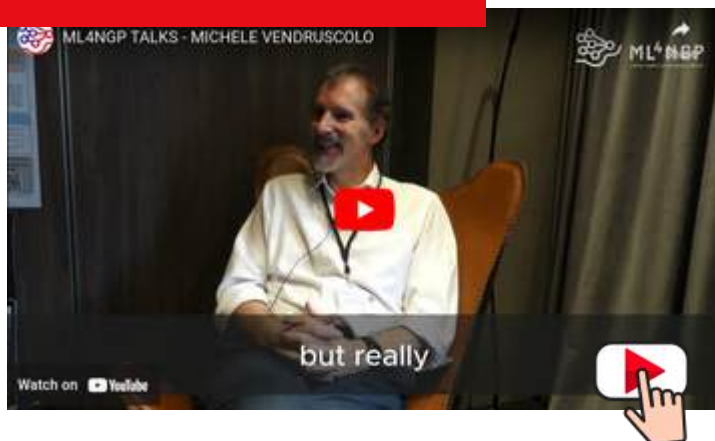
The ML4NGP TALKS are a series of insightful and exclusive interviews with leading researchers, exploring the future of machine learning applications in the study of non-globular proteins. In our first episode, we were honoured to host Prof Michele Vendruscolo, who shared insights into the prediciton of non-globular protein structures using machine learning-based computational tools, and how these innovations are advancing our understanding of molecular interactions and cellular functions
Coming soon, a fascinating conversation with Prof Christine Orengo!

PUBLICATIONS

Garcia-Pardo J., Ventura S. Trends Biochem Sci. 2023

Vasović LM, et al., J Cell Biochem, 2023

Mier P, Andrade-Navarro MA. Comput Struct Biotechnol J., 2023

Bartolomé-Nafría, A., et al., Prion, 2024

Bondarev SA, et al., J Mol Biol, 2024

Gavalda-Garcia J., et al., Bioinformatics, 2024

Clementel D., et al., Nucleic Acids Res, 2024.

Mac Donagh J., et al., Int. J. Mol. Sci, 2024

Piovesan, D., et al., Bioinform Adv., 2024

Piovesan, D., et al. Nucleic Acids Res 2024

Attafi, O. A., et al., arXiv (Cornell University), 2024

Mozaffari, S., et al., bioRxiv (Cold Spring Harbor Laboratory), 2024.

Del Conte, A., et al., Nucleic Adic Res, 2024

ML4NGP NUMBERS AT THE END OF THE SECOND GRANT PERIOD

304 Action Members	46 Countries	7 Meetings & Training Events	382 Participants in events
11 Short Term Missions	7 ITC Conference Grants	21 Publications	2 Deliverables

SECOND YEAR IN REVIEW

HOW CAN YOU PARTICIPATE?

CALL FOR WEBINAR AND TRAINING PROPOSALS!

Our Action continues to grow with new members, and we're eager to reach even more people through open initiatives. **ML4NGP Connect** will provide an open platform for experts to share their knowledge and foster collaboration through webinars and training sessions on topics aligned with our network's mission.

If you're interested in leading a session, please fill out the form with details about the proposed topic, target audience, and your availability.
Let's work together to expand our collective expertise in machine learning for non-globular proteins!

APPLICATION FORM ❯

APPLICATIONS COMING SOON

Applications for the Short Term Scientific Missions, ITC Conference Grants and YRI Conferences Grants will open soon!
Stay up to date about the application process and dates on the following links:

CONFERENCE GRANTS ❯

SCIENTIFIC MISSIONS ❯

ML4NGP
MOBILITY & GRANT PROGRAMME
NOV 2024 - OCT 2025
SHORT TERM SCIENTIFIC MISSIONS
ITC CONFERENCE GRANTS
YRI CONFERENCE GRANTS
COMING SOON

These initiatives are part of the activities of the COST Action ML4NGP, CA21160, which is supported by COST (European Cooperation in Science and Technology).

📅 MARK YOUR CALENDARS

February, 2025
3-7
Training School
NMR for Intrinsically Disordered Proteins
#NMR4IDP
📍 Brno, Czech Republic

March, 2025
18-19
Workshop
AlphaFold for Non-globular Proteins
#AF4NGP
📍 Barcelona, Spain

May, 2025
20-23
Meeting
Machine Learning for Non-globular Proteins
#ML4NGP
📍 Vilnius, Lithuania

APPLICATIONS