# NEWSLETTER

DECEMBER 2025 ML4NGP COST ACTION | ED. 4

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Group photo at 3rd ML4NGP Main Meeting, in Vilnius, Lithuania.

We are pleased to share the fourth edition of the ML4NGP newsletter, marking a strong and dynamic third year of our COST Action. Over the past grant period, the ML4NGP community continued to grow and consolidate, bringing together researchers across disciplines to advance the understanding of **non-globular proteins** through **machine learning** and **integrative approaches**. In this edition, we highlight key milestones including the 3rd ML4NGP Meeting in Vilnius, our hands-on Training School in Brno, targeted workshops, and expanded mobility and training opportunities supporting early-career researchers.

A key scientific milestone of this grant period was the preparation of a joint letter published in Open Research Europe, co-written with the Scientific Advisory Board, reflecting on the **2024 Nobel Prizes in Chemistry and Physics** and their impact on computational and protein sciences, underscoring the relevance and visibility of the ML4NGP COST Action mission and goals.

This edition also highlights the outreach and community-building initiatives, including joint **publications, ML4NGP Talks** and **ML4NGP Connect**, which continue to foster dialogue across experimental, computational, and theoretical frameworks as we move confidently toward the last year of the Action.

## TOP NEWS

### ML4NGP Meeting 2025 in Vilnius

Strengthening a unified scientific community at the intersection of machine learning and non-globular protein research, through high-level scientific exchange and collaboration.

### ML4NGP Go Global: support scientific mobility

Empowering early-career researchers through international mobility, training, and conference participation, fostering career development and cross-border collaboration.

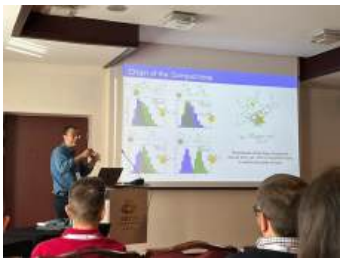
### Connecting between talks and seminars

Opening the dialogue through interviews and seminars with leading experts, bridging experimental, computational, and theoretical perspectives in NGP research.

# THIRD YEAR IN REVIEW

## ML4NGP MAIN MEETING 2025

From May 20–23, 2025, over 100 researchers from 31 countries came together in the historic old town of Vilnius for the 3rd ML4NGP Meeting, a vibrant hub for cutting-edge research at the intersection of machine learning and non-globular protein science. The four-day programme featured inspiring keynote talks, high-quality scientific presentations, and lively poster sessions covering topics from intrinsically disordered proteins (IDPs) and low-complexity regions to advanced ML-integrative methods and experimental techniques like NMR and smFRET.




Vibrant atmosphere and moments of sharing and exchange of knowledge during the 3rd ML4NGP Main Meeting, in Vilnius, Lithuania.

Beyond scientific talks, the meeting fostered deep engagement through working group sessions, collaborative discussions on mid-term goals, and a first-of-its-kind round-table on "Challenges and Opportunities in NGP Research", bringing together voices from academia, industry, and tech transfer. The open and collaborative spirit underscored the diversity of the ML4NGP community and set the stage for sustained innovation and future collaborations.

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## TRAINING SCHOOL

The 3rd ML4NGP Training School, held at CEITEC in Brno, brought together early-career researchers and leading experts for a week of intensive theoretical and practical training focused on **NMR spectroscopy and its applications to intrinsically disordered proteins (IDPs)**. Through an interactive program of lectures coupled with hands-on sessions, participants dived from foundational NMR principles to more advanced topics such as J-coupling, relaxation techniques, NOE for structural characterization, EPR, and cutting-edge methods for studying complex biomolecular challenges. Through expert guidance and unique interdisciplinary connections, this event deepened technical skills, and equipped the next generation of scientists with tools to advance research in machine learning and non-globular protein science.

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Group photo with participants attending the 3rd ML4NGP Training School.

# THIRD YEAR IN REVIEW

## WORKSHOP

The ML4NGP Workshop on "Resources and infrastructure to explore the continuum between globular and non-globular proteins" took place as a pre-event of the Elixir 3DBioinfo 2025 meeting providing an excellent opportunity to discuss the challenges and opportunities in exploring the continuum between globular and non-globular proteins, including IDPs, tandem repeat proteins, protein aggregation, and much more.

Group photo with participants at the ML4NGP Workshop in Barcelona.

The workshop brought together 28 participants from xx countries, who focused the discussion on identifying commonalities and fostering synergies among the key resources and databases used for globular and non-globular proteins. The workshop paved the way for the drafting of a community paper aimed at cautioning scientists against uncritically accepting AlphaFold results.

## MOBILITY AND TRAINING

### ML4NGP GO GLOBAL IN 2025: SHORT SCIENTIFIC MISSIONS AND CONFERENCE GRANTS

During the third grant period, five conference grants were awarded to young researchers and ITC members and four short term scientific missions were supported for mobility and training of researchers among different countries and institutions. These funding opportunities support not only the scientific research and foster collaboration among the Action's members but also contribute for personal growth and institutional capacity-building.

**Scientific Missions**

David Tuzincin
Czech Republic ✈ Switzerland

Mahta Mehdiabadi
Italy ✈ Denmark

Viktor Bartošík
Czech Republic ✈ France

Hamidreza Ghafouri
Italy ✈ France

**Conference Grants**

Ana Melo
Portugal ✈ USA

Claire Buchanan
Spain ✈ UK

Andrius Sakalauskas
Lithuania ✈ Sweden

Jovana Kovačević
Serbia ✈ UK

Emre Aktas
Turkey ✈ Czech Republic

## ML4NGP NUMBERS AT THE END OF THE THIRD GRANT PERIOD

| | | |
|---|---|---|
| 321 Action Members | 46 Countries | 382 Participants in events |
| 15 Short Term Missions | 14 Conference Grants | 10 Meetings & Training Events |
| 26 Publications | 4 Deliverables | 9 Talks and seminars |

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# THIRD YEAR IN REVIEW

## ML4NGP TALKS

The ML4NGP Talks series expanded with six in-depth interviews featuring leading experts in non-globular protein research.

In the last episodes, we explored the central role of experimental techniques, particularly nuclear magnetic resonance (NMR), in understanding the dynamics, interactions, and biological relevance of intrinsically disordered proteins, while also highlighting the continued need for deep theoretical expertise alongside integrated biological perspectives. It was highlighted the growing impact of machine learning and computational approaches in mapping protein diversity, studying protein–protein interactions, and uncovering new functional families, emphasizing complementarity between experimental and AI-driven methods.







The invited speakers also share their reflections on scientific career paths, mentorship, and the importance of attracting and training the next generation of specialists, making the ML4NGP Talks a rich platform for both scientific insight and community reflection.

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## ML4NGP CONNECT

As part of the ML4NGP Connect series, a collaborative platform for sharing expertise at the intersection of machine learning and non-globular proteins, we recently hosted three engaging seminars with leading scientists. Prof. Michele Vendruscolo and Dr. Zsuzsanna Dosztányi kicked off the series with talks on cutting-edge topics in intrinsically disordered proteins and structural bioinformatics, respectively.

Prof Dr Joana Pereira later explored deep learning, network analysis, and computational workflows for revealing protein diversity and novel functional classes.

These seminars brought together emerging perspectives from theory, computational and experimental framework to support knowledge exchange across and beyond the ML4NGP community.

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# THIRD YEAR IN REVIEW

## PUBLICATIONS

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