

Moving Beyond Memorisation

Resources for Generalisable Protein Complex Prediction

P(L)INDER training workshop



plinder

The Protein-Ligand Interaction
Dataset and Evaluation Resource

more data
more diversity
more flexible



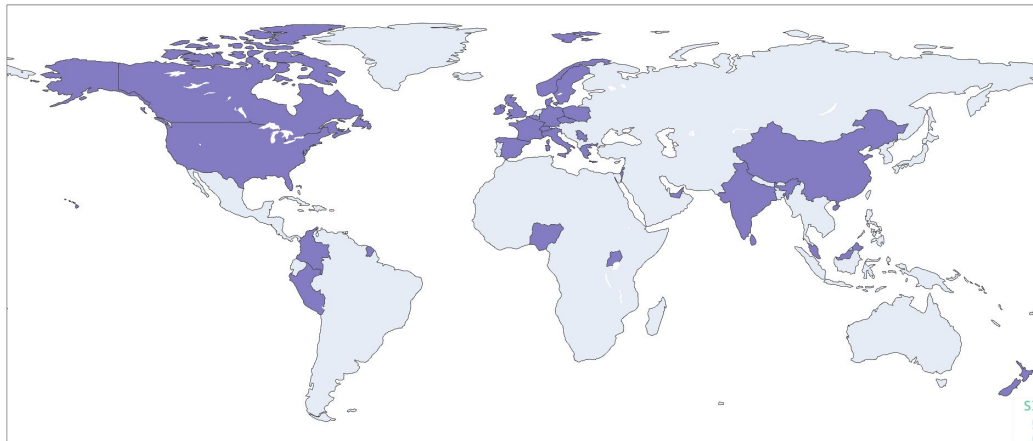
pinder

The Protein Interaction
Dataset and Evaluation Resource

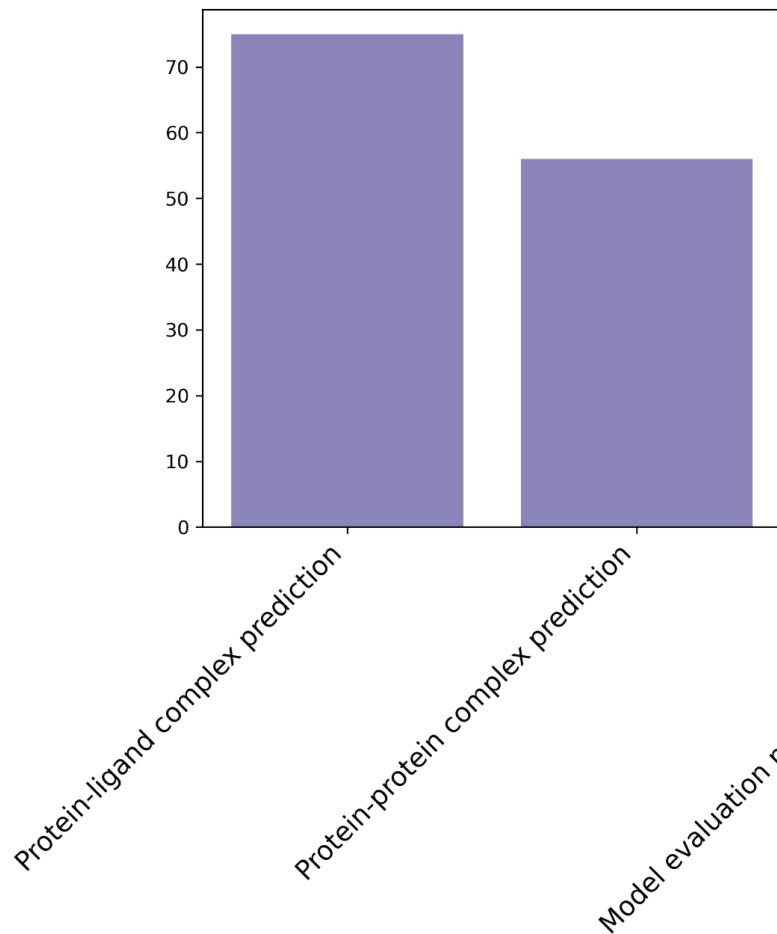
higher quality
less leakage
better evaluation

2024-09-24

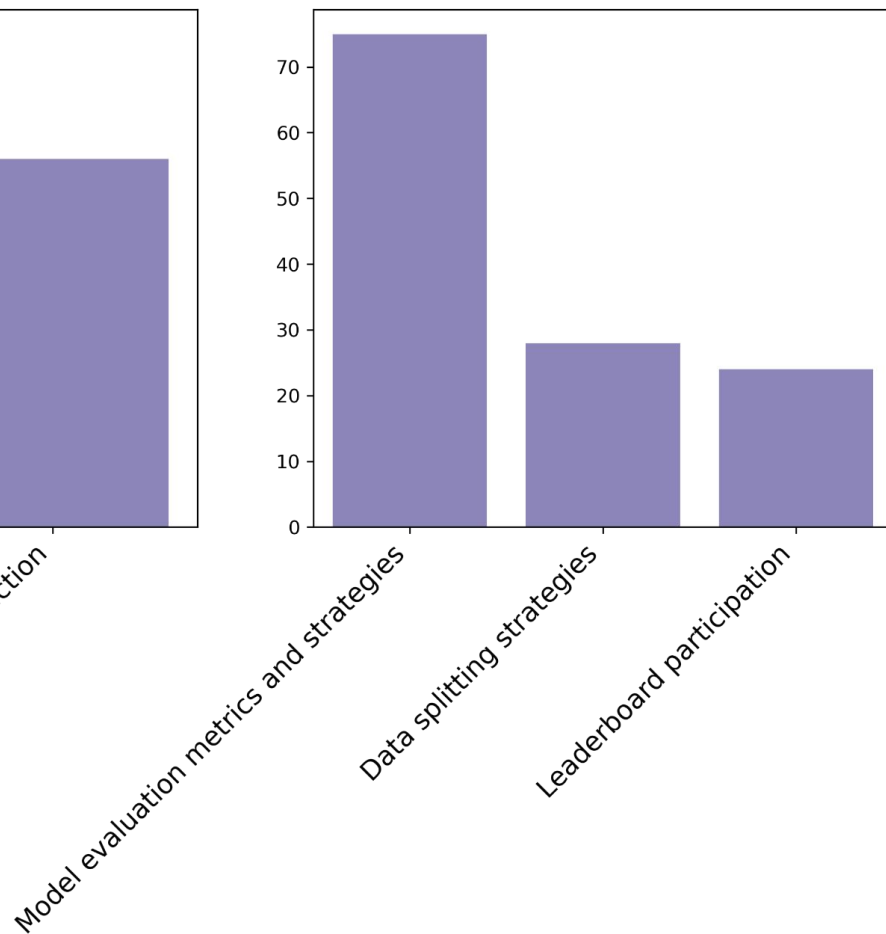
Over 150 registrations from 30 countries



Which area is more relevant to you?



Which topic is of particular interest to you?



Key Housekeeping Points

Workshop scope: how to use P(L)INDER for training and evaluating models for complex prediction, not about specific proteins/ligands.

Session Recordings: In response to numerous requests, we will record the sessions to make them available on-demand, most likely on the SIB YouTube channel.

Slides and Notebooks: These are available at https://github.com/plinder-org/moving_beyond_memorisation

Keep your microphones muted: unless presenting to avoid background noise during sessions.

Live Interaction: We encourage questions, discussions, or feedback during the workshop. Use our dedicated Discord P(L)INDER User Group: <https://discord.gg/KgUdMn7TuS>

Technical Support: if you encounter any technical difficulties during the workshop, ask for assistance on the Discord server in the “tech-support” channel for real-time help.

Workshop schedule

15:00 - 15:15 *Welcome and introduction* - Leila

15:15 - 16:00 *Connected concepts in datasets, benchmarking and training* - Jay

16:00 - 16:35 *Metrics for measuring protein and complex model accuracy* - Xavier and Gabriel

16:35 - 16:40 *Intro to dataset presentations and splitting into two groups* - Jay

16:40 - 17:00 Break

17:00 - 18:30 Parallel sessions

PINDER dataset for PPI prediction - Danny and Mehmet

PLINDER dataset for PLI prediction [another zoom link] - Vladas, Tom and Yusuf

18:30 - 19:00 Break

19:00 - 20:00 *Hugging Face models and leaderboard submission* - Simon

20:00 - 20:20 *Feedback and next steps* - Jay

20:20 - 20:30 *Closing remarks* - Leila