Moving Beyond Memorisation Resources for Generalisable Protein Complex Prediction

P(L)INDER training workshop



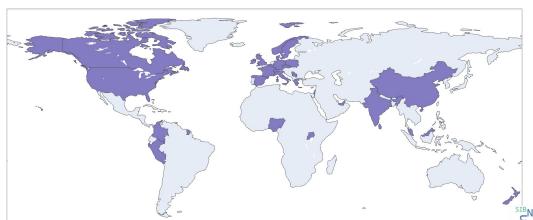
The Protein-Ligand Interaction Dataset and Evaluation Resource

> more data more diversity more flexible

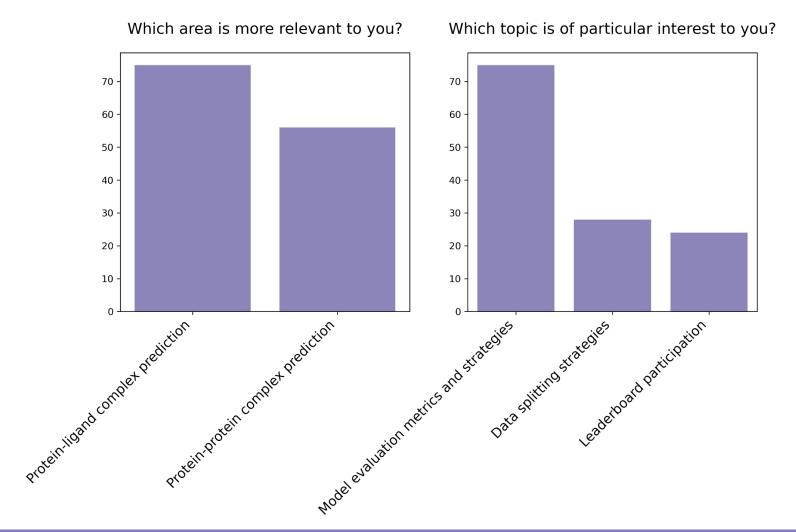
The Protein Interaction Dataset and Evaluation Resource

higher quality less leakage better evaluation

Over 150 registrations from 30 countries



SIBNOSTRUM SCULLA STARLED STITUTE Norwegian National Hedden Amazon Size Northwestern academia Therapeutics Productiver Student Sound National Student Student



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.

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 Danny and Mehmet
- **16:40 17:00** Break
- 17:00 18:30 Parallel sessions

PINDER dataset for PPI prediction [another zoom link] - Danny and Mehmet

PLINDER dataset for PLI prediction - 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