

Machine Learning-based prediction of protein-ligand binding affinity

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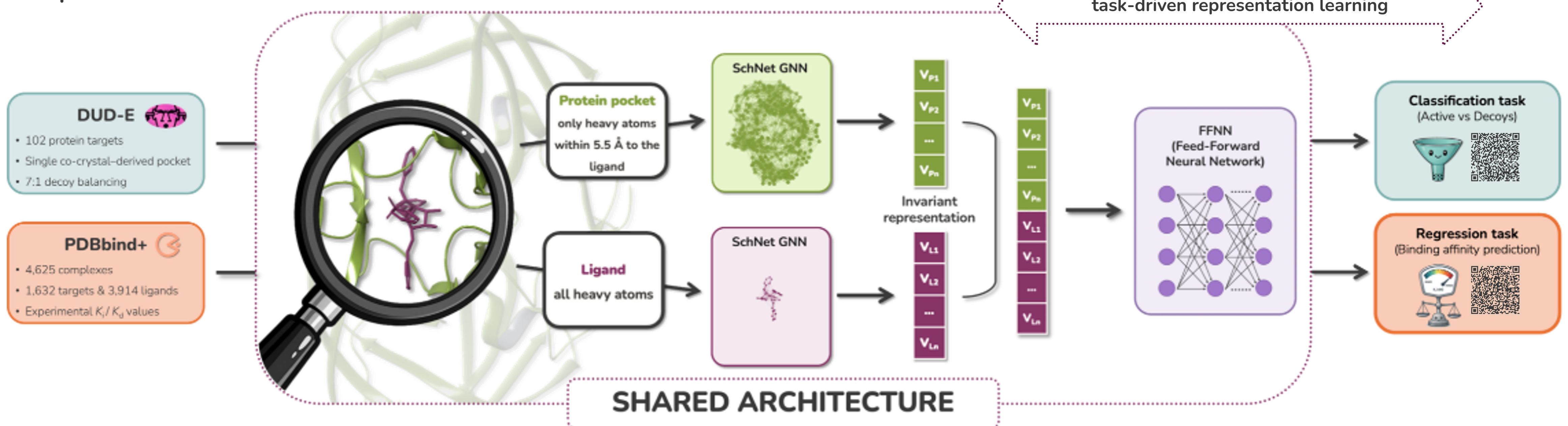
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drug discovery; binding affinity prediction; machine learning; deep learning; graph neural networks

SUMMARY

Predicting **protein–ligand binding affinity** is a key challenge in **computational drug discovery** for compound prioritization. **Machine learning** provides a scalable alternative to traditional experimental and in silico approaches. Here, we propose a **two-stage machine learning framework** that **does not require protein–ligand complex structures**.



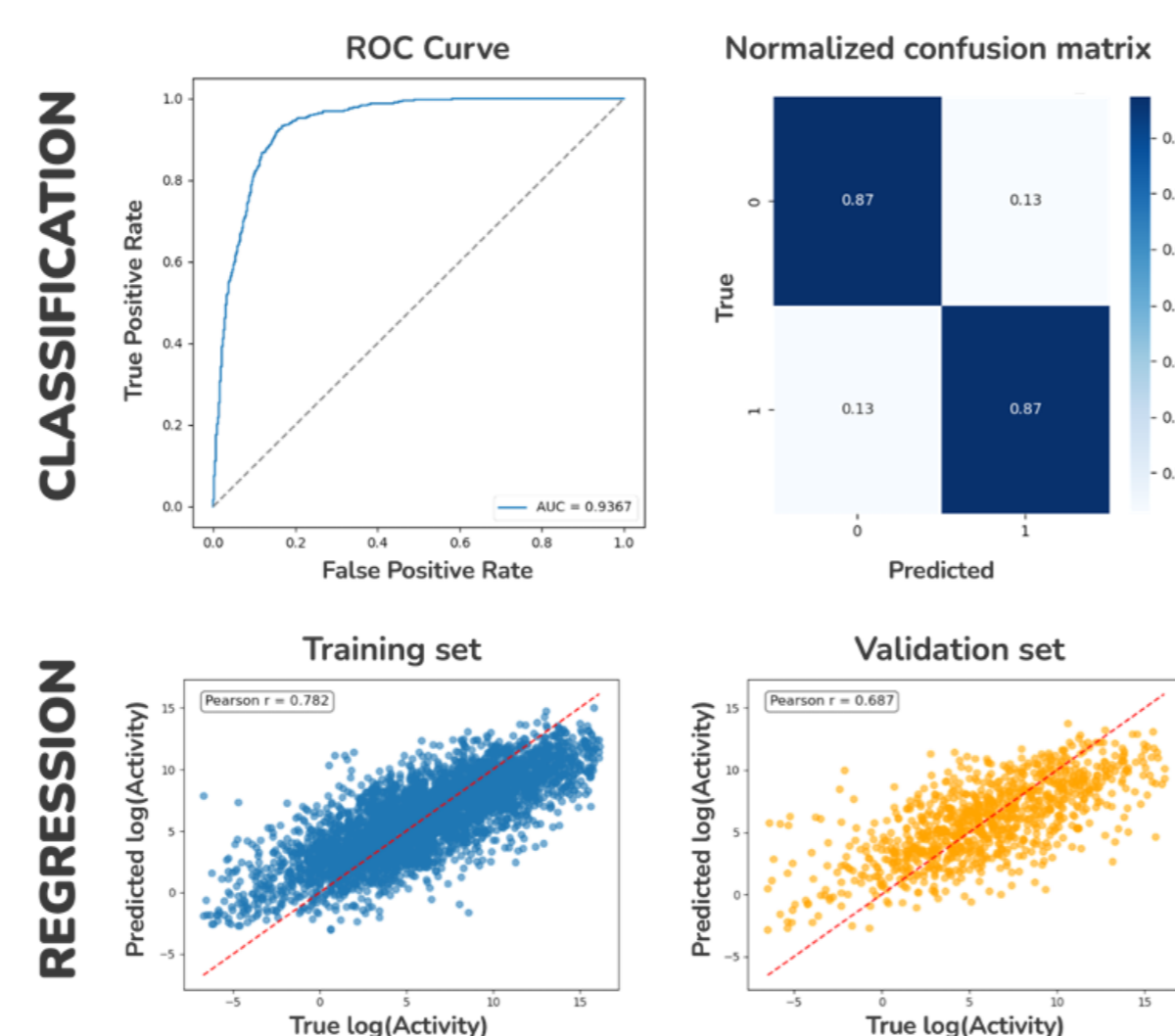
THE ALGORITHM

Classification and regression models share a **common architecture** and are trained **end-to-end** via backpropagation using the Adam optimizer and task-specific loss functions.

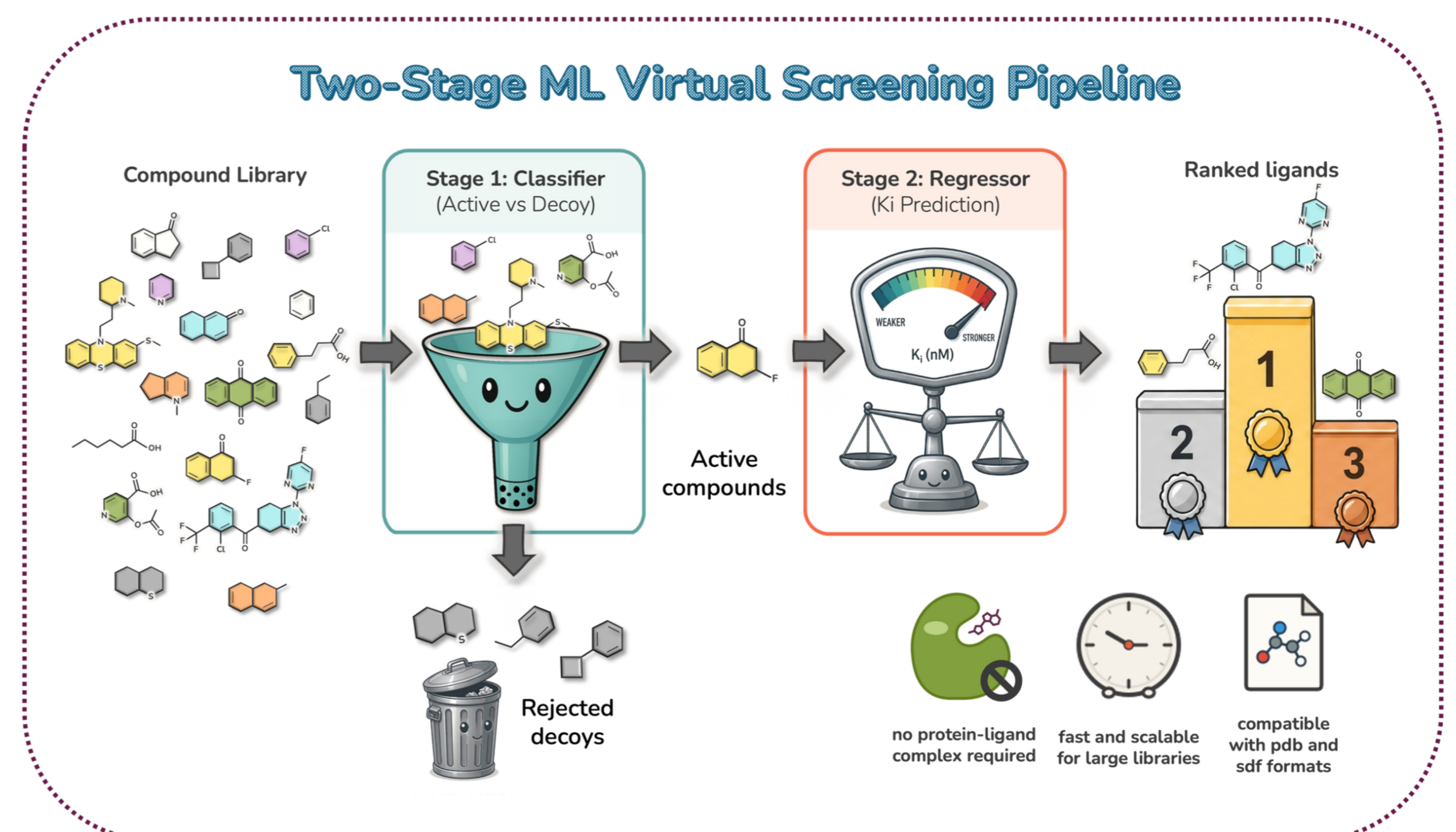
VALIDATION

STRONG OVERALL PERFORMANCE

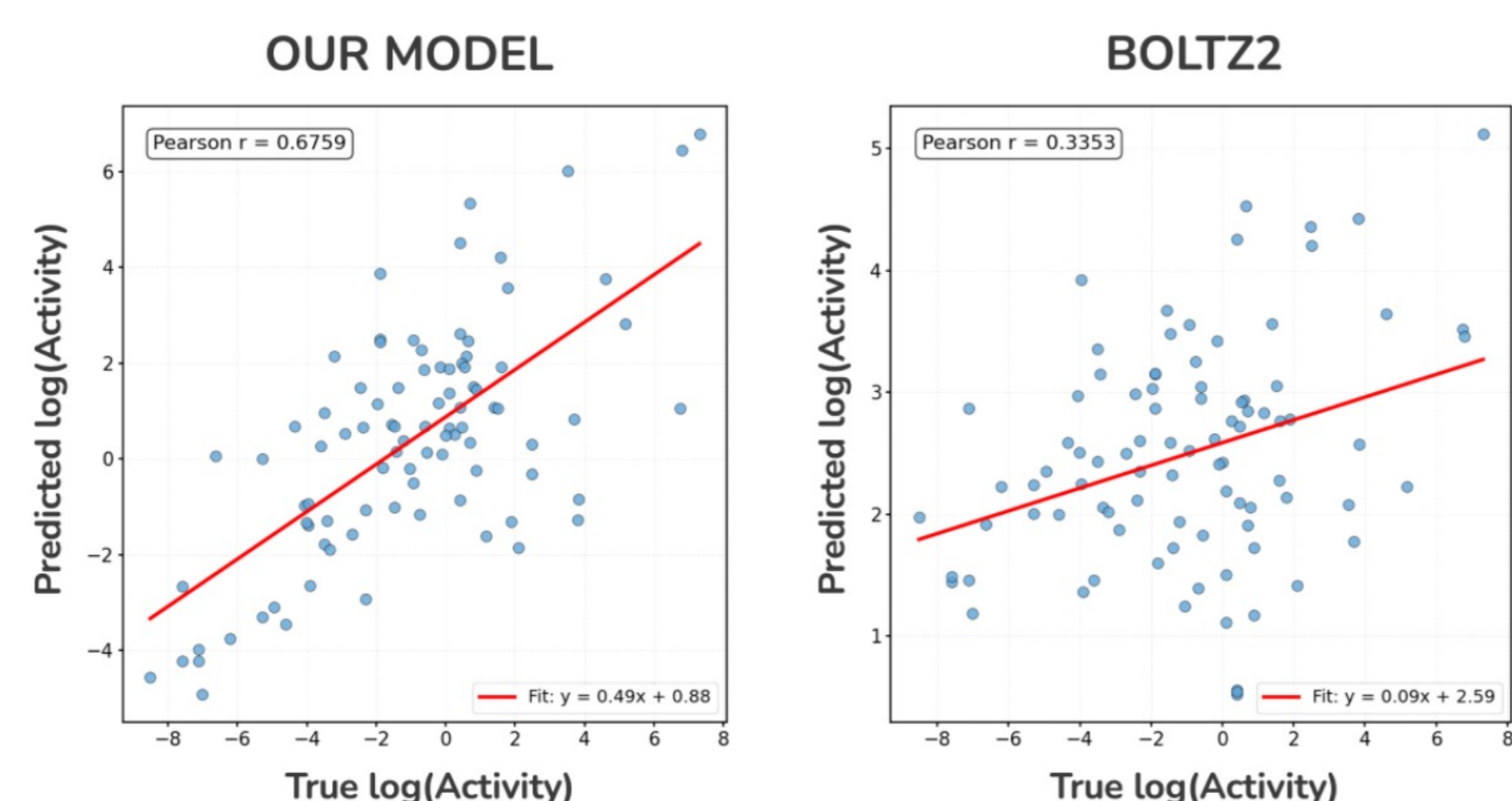
- ✓ ROC AUC ≈ 0.99
- ✓ balanced accuracy ≈ 0.87
- ✓ R^2 training ≈ 0.78
- ✓ R^2 validation ≈ 0.69



THE PIPELINE



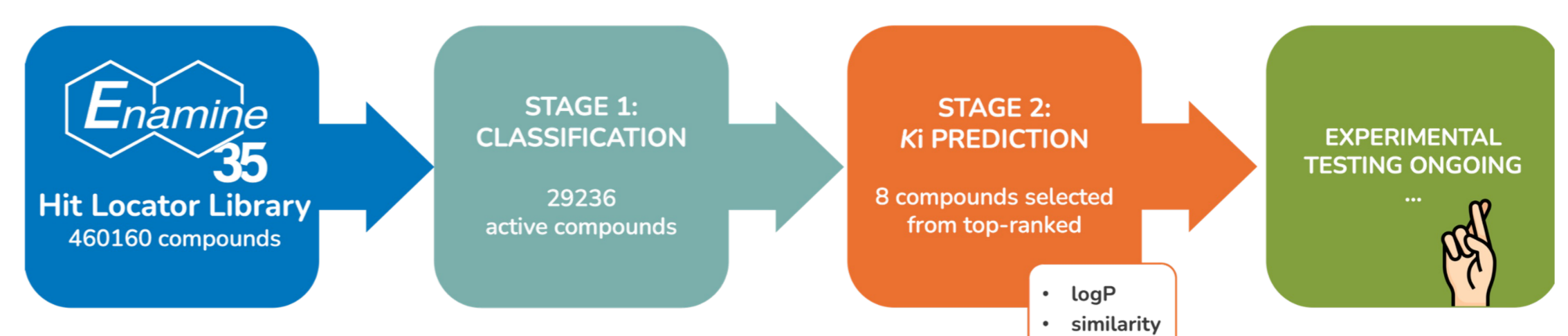
EXTERNAL VALIDATION ON HIV-1 PROTEASE



THE CASE STUDY

VIRTUAL SCREENING AND K_i PREDICTION FOR ENAMINE LIBRARY

Target: HIV-1 PROTEASE



AKNOLEDGMENTS

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