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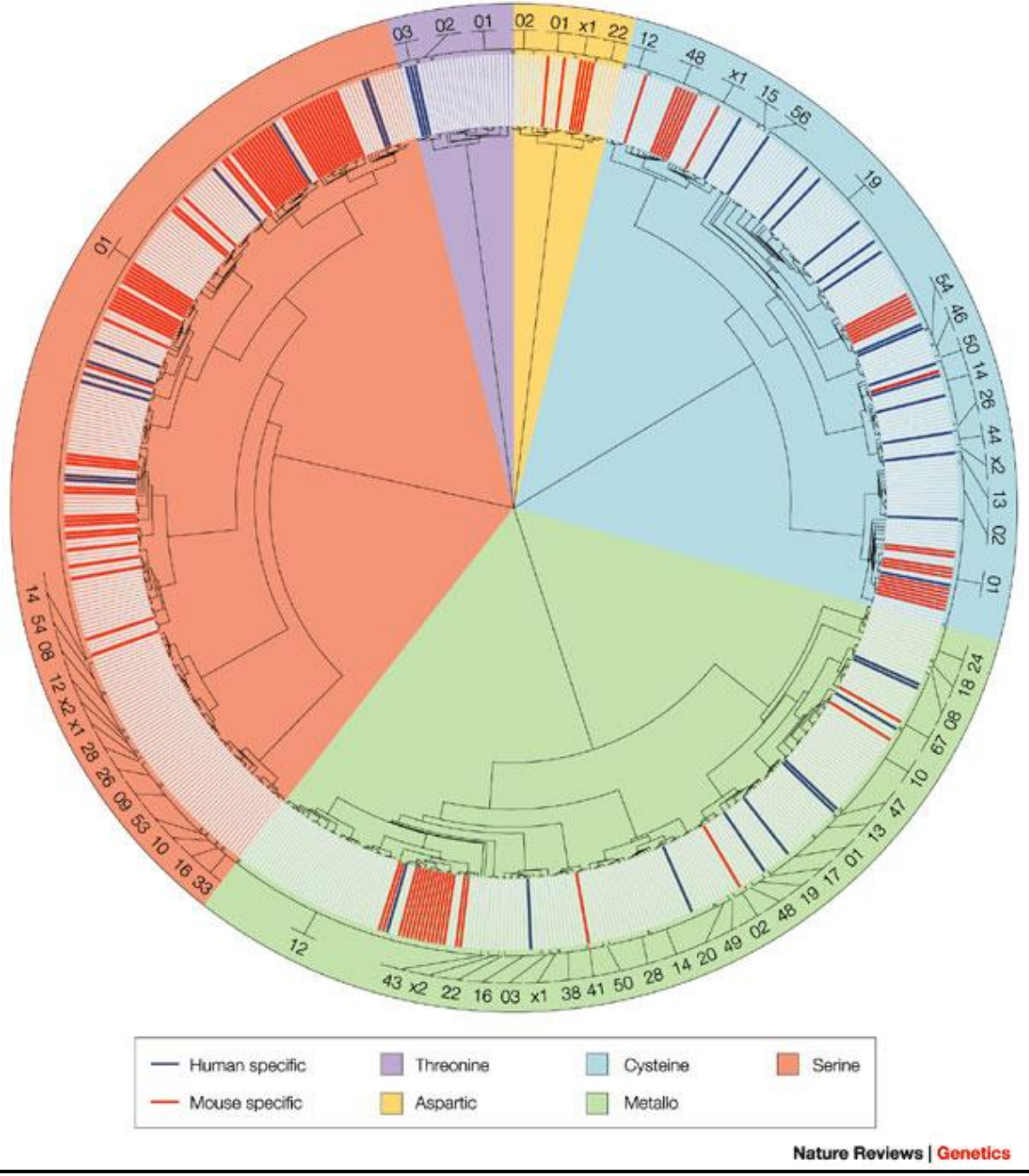
MODELING OF SERINE PROTEASE SUBSTRATE CATALYSIS IN SYNTHETIC MICELLE ENVIRONMENT

PROJECT OVERVIEW

Our goal is to predict and understand how serine proteases catalyze reactions inside synthetic micelles using a hybrid machine learning and simulation pipeline.

- Background
  - Inspired by catalytic processes inside micellar systems synthesized by Professor Yan Zhao's lab. We are further analyzing it to gain insight on what this data could help future researchers predict.
- Why is it important?
  - This links enzymatic chemistry, micelle-based encapsulation, and AI/Ml prediction can help within drug design.



UNDERSTANDING THE BASICS

PARAMETER	WHAT IT REPRESENTS	ACTIVATOR EFFECT
K_{cat}	Turnover number: number of reactions per enzyme per second	↑ with activators that stabilize the transition state or catalytic residues
K_m	Substrate concentration at half-max velocity	↓ with activators that improve binding affinity or orientation
K_{cat}/K_m	Catalytic efficiency (best overall measure)	↑ with both improved binding and enhanced turnover

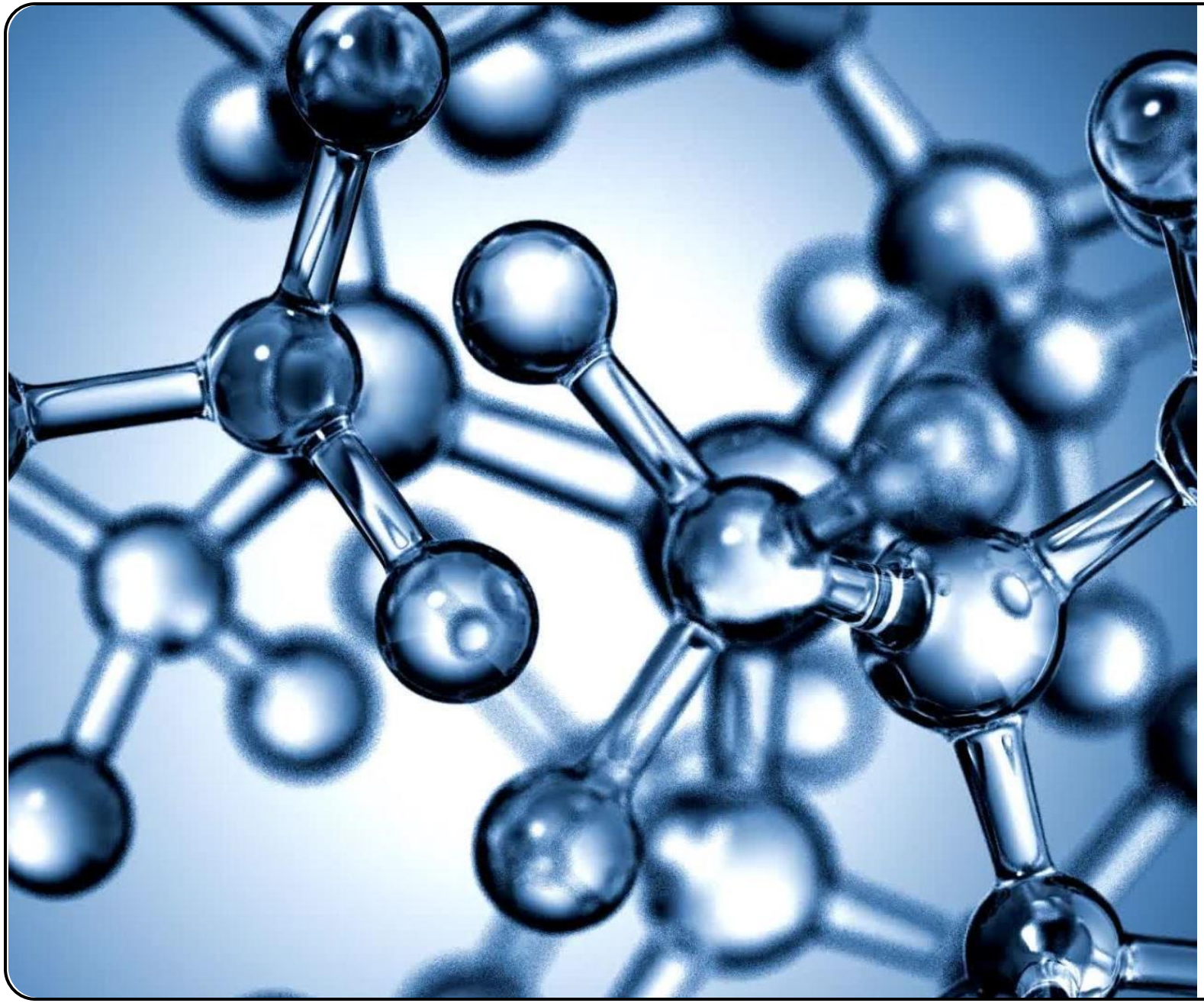
MY ROLE

Curating enzyme-substrate data of activators

Performing molecular docking to identify binding poses

Training graph neural networks on structural data

Running simulations of catalysis in micellular environments

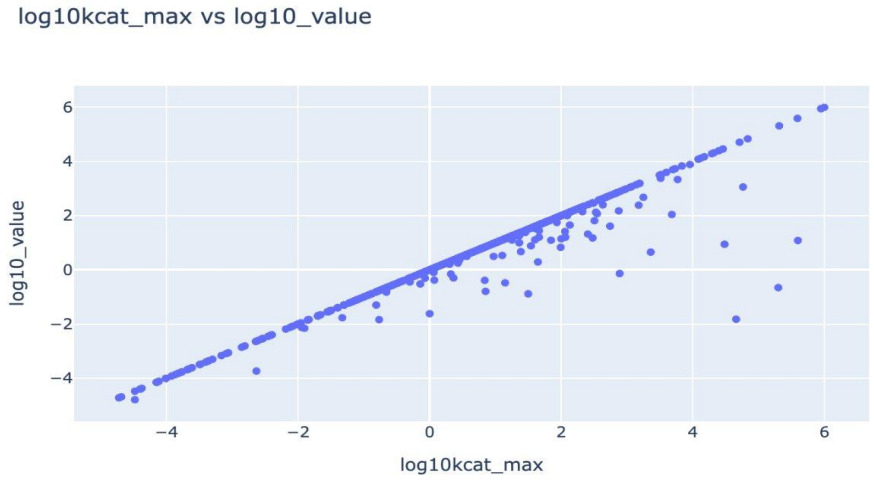


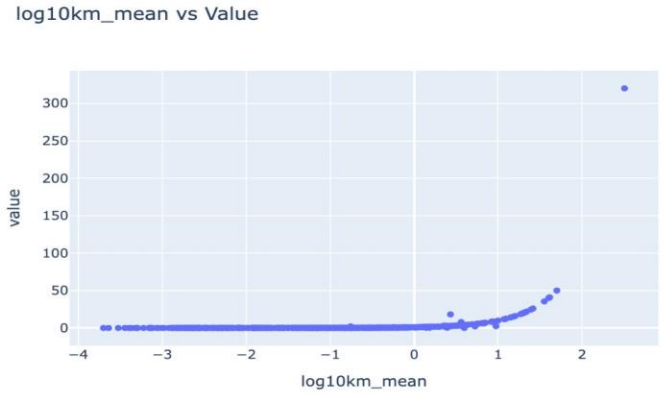
WHAT I'VE LEARNED

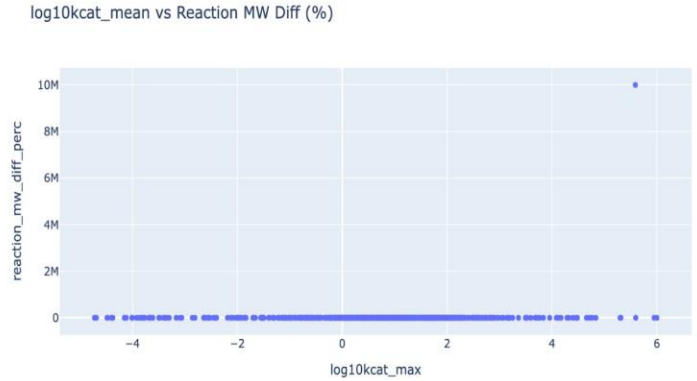
Hands-on experience with:

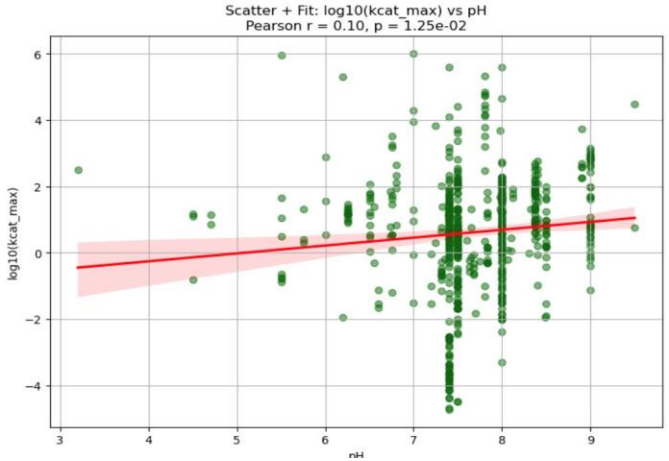
- Protein-ligand docking (AutoDock / PyMOL)
- Representing molecules via SMILES + graph structures
- Implementing GNNs and transfer learning strategies

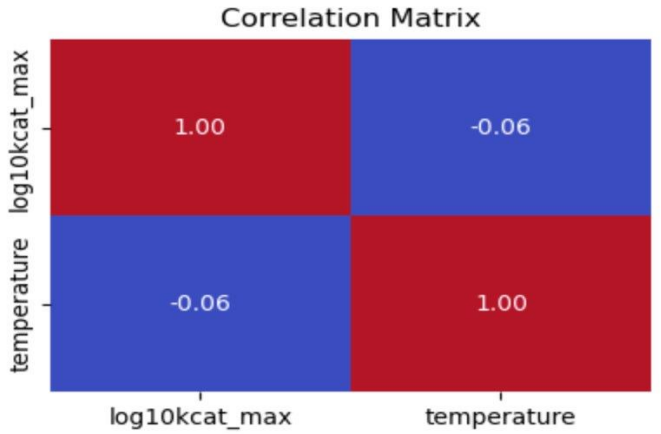
Micellar encapsulation theory and enzymatic catalysis











PROGRESS SO FAR...

CURRENT CHALLENGES

- Lack of consistent labeled data on catalytic efficiency in micelles
- Complexity of simulating micellar environments computationally
- High computational cost of MD + ML integration
- Docking artifacts due to static structures

GOALS FOR THE REMAINDER OF THE SUMMER

1. Finish deep learning molecular docking
2. Integrate ML predictions with MD simulations
3. Validate predictions against experimental kinetic data
4. Explore the influence of micelle polarity/size on catalysis

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