Deep learning from deep mutagenesis: understanding and engineering molecular specificity

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Deep learning from deep mutagenesis

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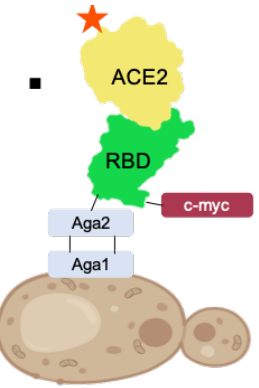
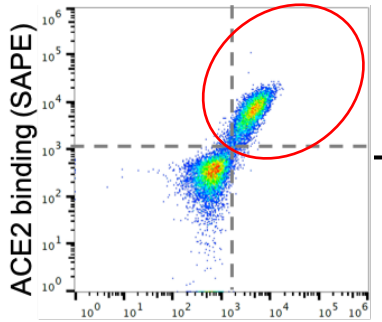
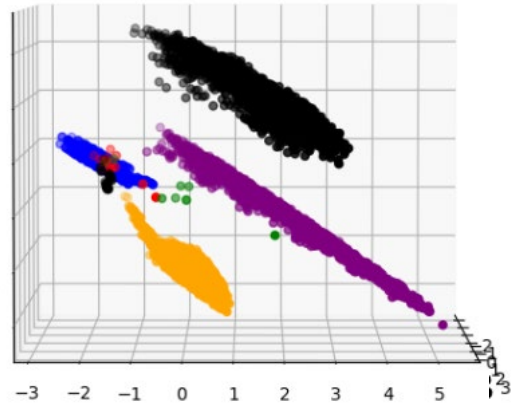
- Specificity of molecular recognition is critical in biology and therapeutics.

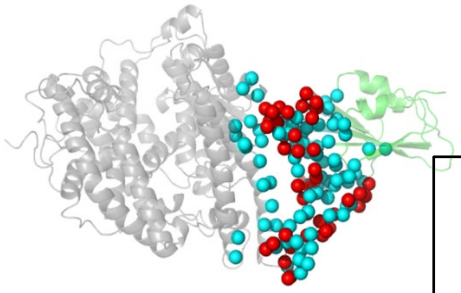
Prediction of sequence degeneracy in interactions is a fundamental question in biology. Can we forecast variation of key protein-protein interactions?



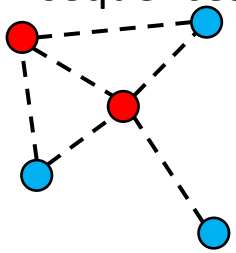




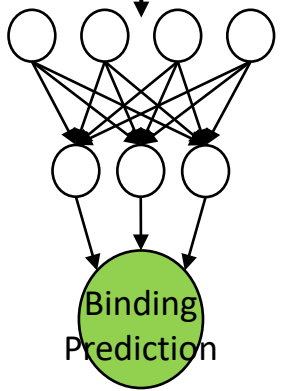
Mutagenized interface



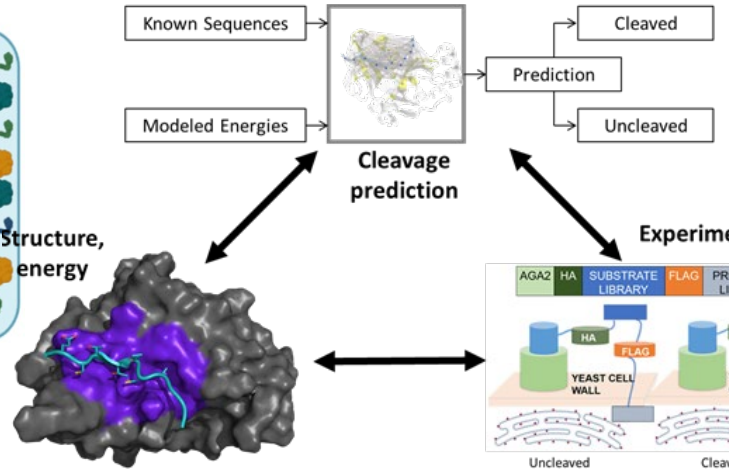
Deep sequence;
~ 1 million sequences

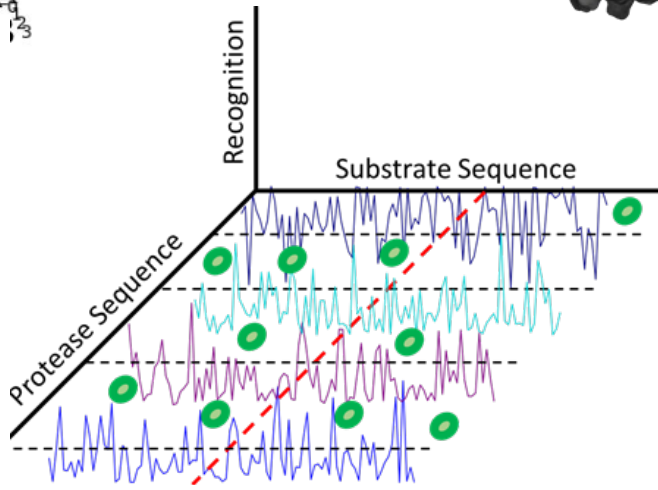


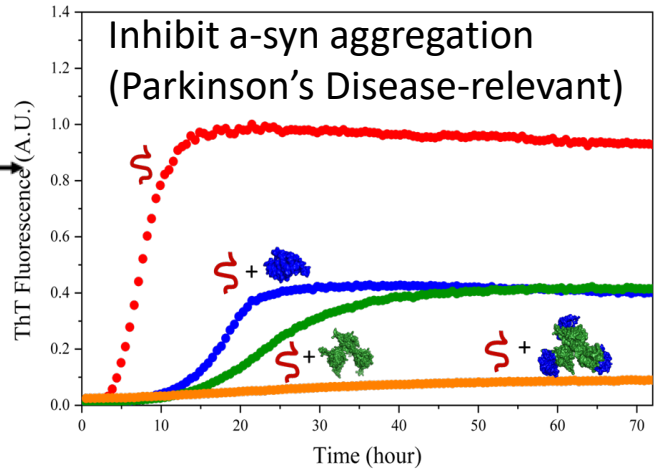
Node, Edge, physics-derived features



Precise editing of proteins: CRISPR for proteome
Spatial, temporal control; specificity criticial







With Jean Baum

Self-driving lab for for generating and improving designed enzymes using robotics and AI

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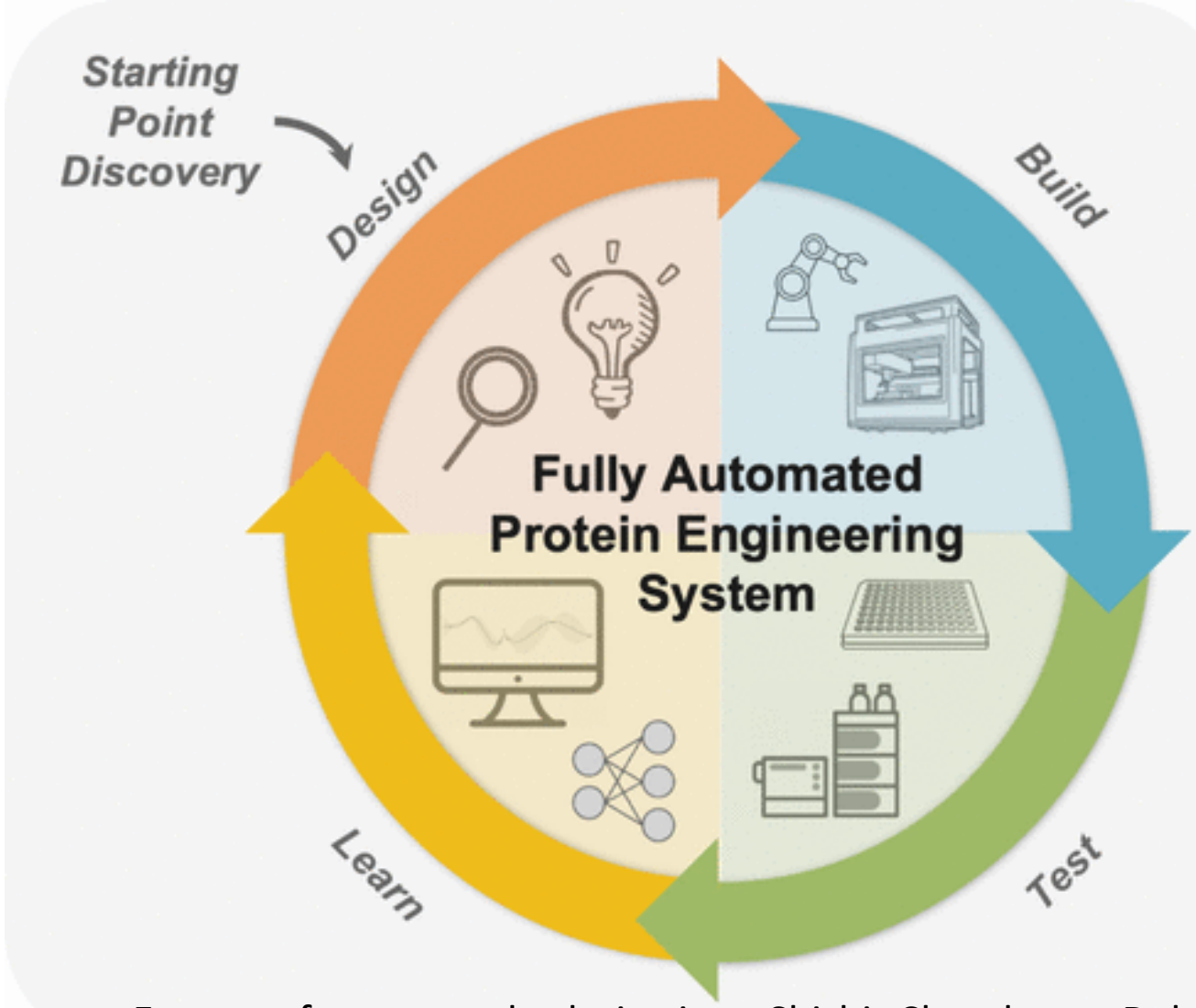

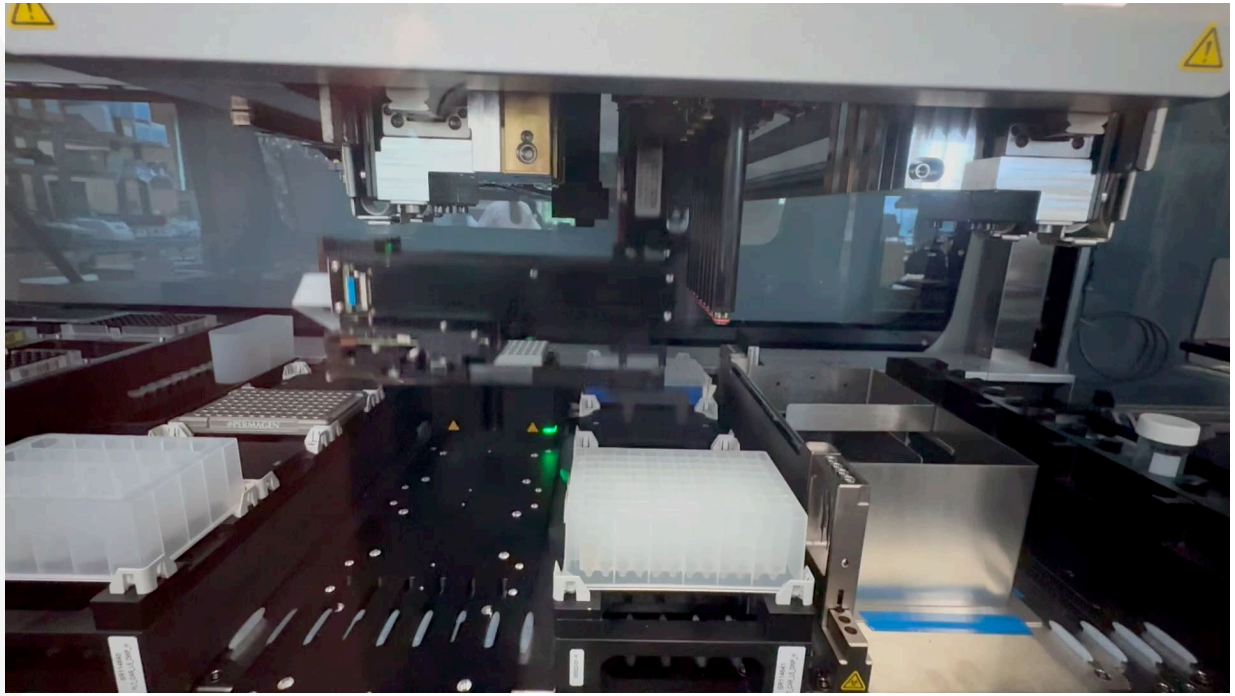

"Eventually, much of science will be conducted at 'self-driving labs'—automated robotic platforms combined with artificial intelligence. Here, we can bring AI prowess from the digital realm into the physical world".
- Eric Schmidt, MIT Tech Review 2023

Enzymes for seaweed valorization - Shishir Chundawat, Debashish Bhattacharya, Jose Avalos (Princeton)

How to design and learn effectively from data (agents, fine-tuning?) via HPC workflows - with Shantenu Jha, NAIRR pilot