



## **Problem: AI for Molecular Simulations and Drug Design**

- **Extract Features, Predict Emergent Properties from Large amounts of MD Data on Complex Biological Systems.**

datasets: large databases of atomic coordinates, velocities, chemical relationships

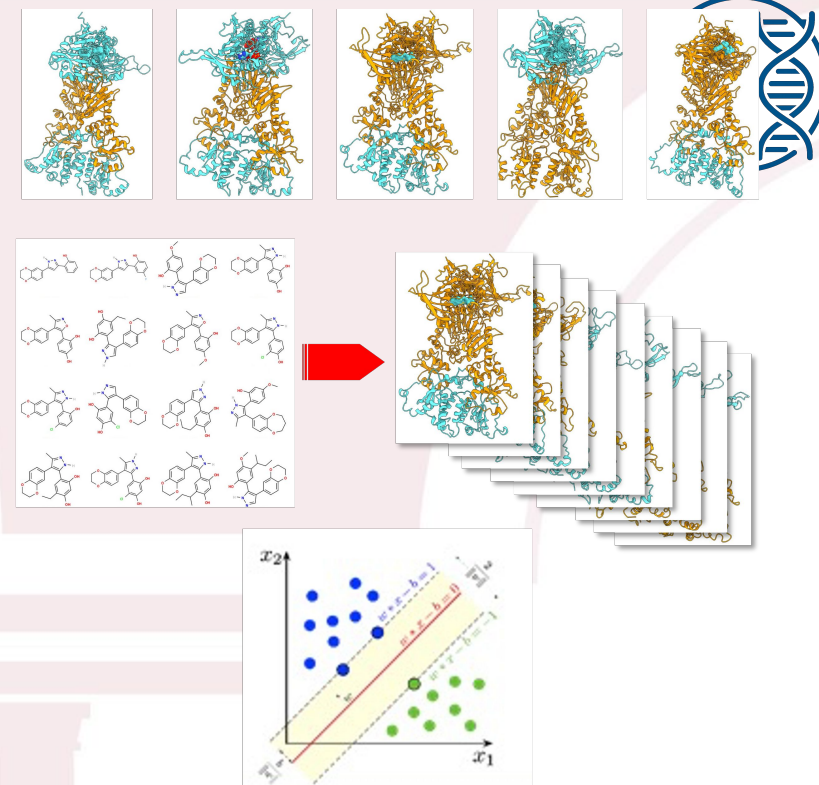
- **Generative Design of Small Molecules with Pharmacological Activities; Integration with Knowledge on Systems Dynamics.**

datasets: Ultra-Large Compound Libraries (Million Compounds with annotated properties)



# Call for Help

- Identify/Develop the Best AI Algorithm/Approach for Identification of Emergent Properties from MD Simulations.



- How to Combine Generative Approaches with MD-based Information and Chemical Sense/Rules to Develop Small Molecules.

