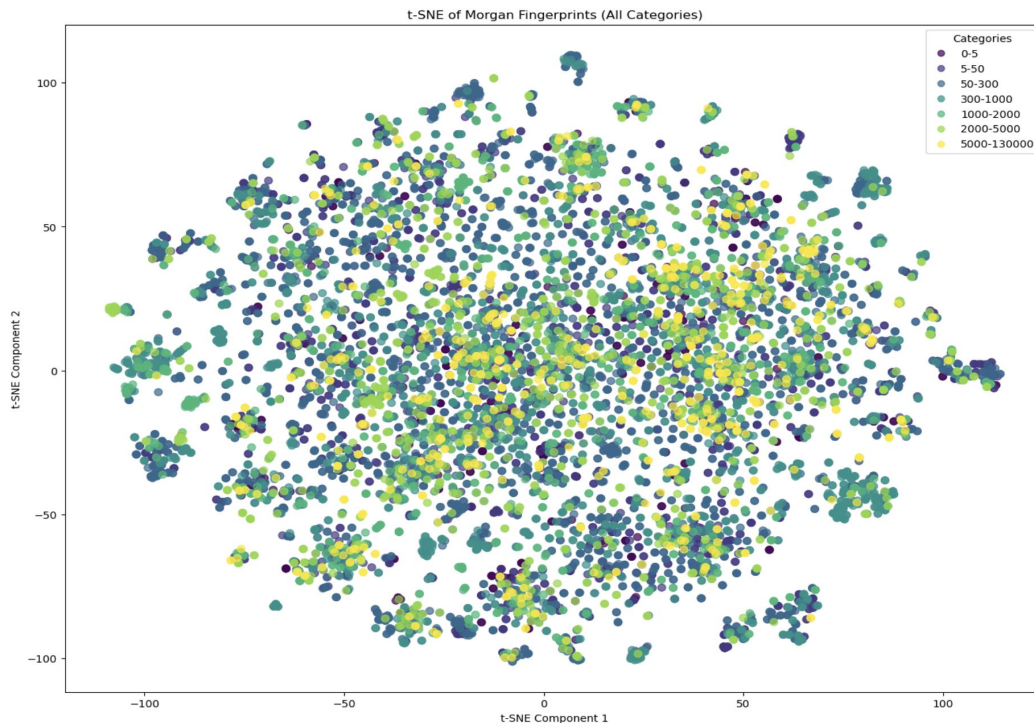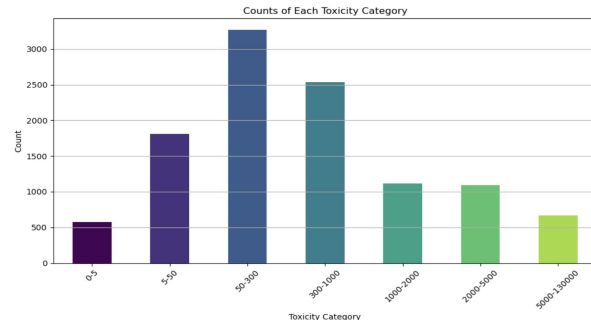# What I've Done

Lab: predicting toxicities of compounds

- Papers
  - Deeptox
  - TOXRIC
- Tutorials
  - Pytorch
  - Torchdrug
  - 3B1B videos
- Analyzed toxicity data
  - T-SNE of Morgan fingerprint of chemicals toxic to rats, colored by LD50 value



Counts of Each Toxicity Category



t-SNE of Morgan Fingerprints (All Categories)

# What I Will Do

Start training models to predict toxicity

- Data: largest TOXRIC dataset
    - Same species, administration method, system affected
    - Pro: Avoid confusing the model
    - Con: Might be too little data (35,000 lines)
- Compare different models
- Simple SMILES Transformer
    - Out of the box regression training
    - Modify it to classification, toxicity cutoff LD50 = 5000?
- Torchdrug (GNN)
- Dtox (MLP)