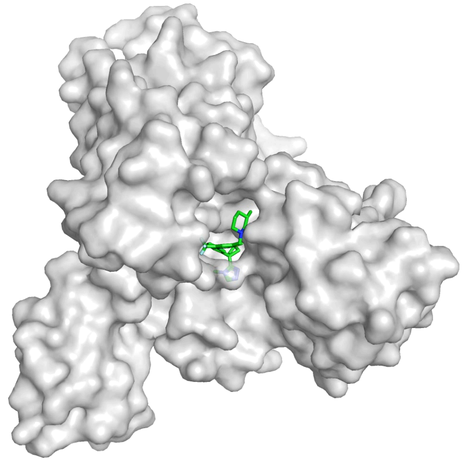
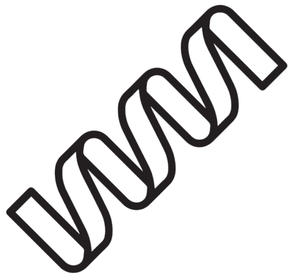
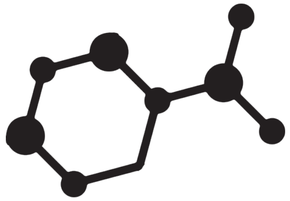
CACHE Challenge 4

Discover new drugs for cancer immunotherapy

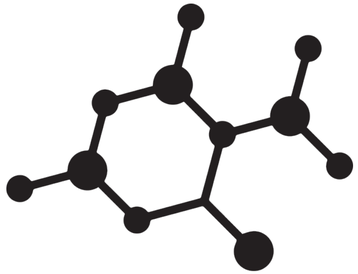




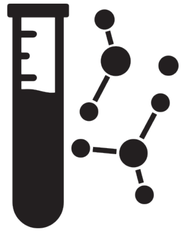
1. Identify a protein target



2. Find molecules that bind to target



3. Optimize molecules



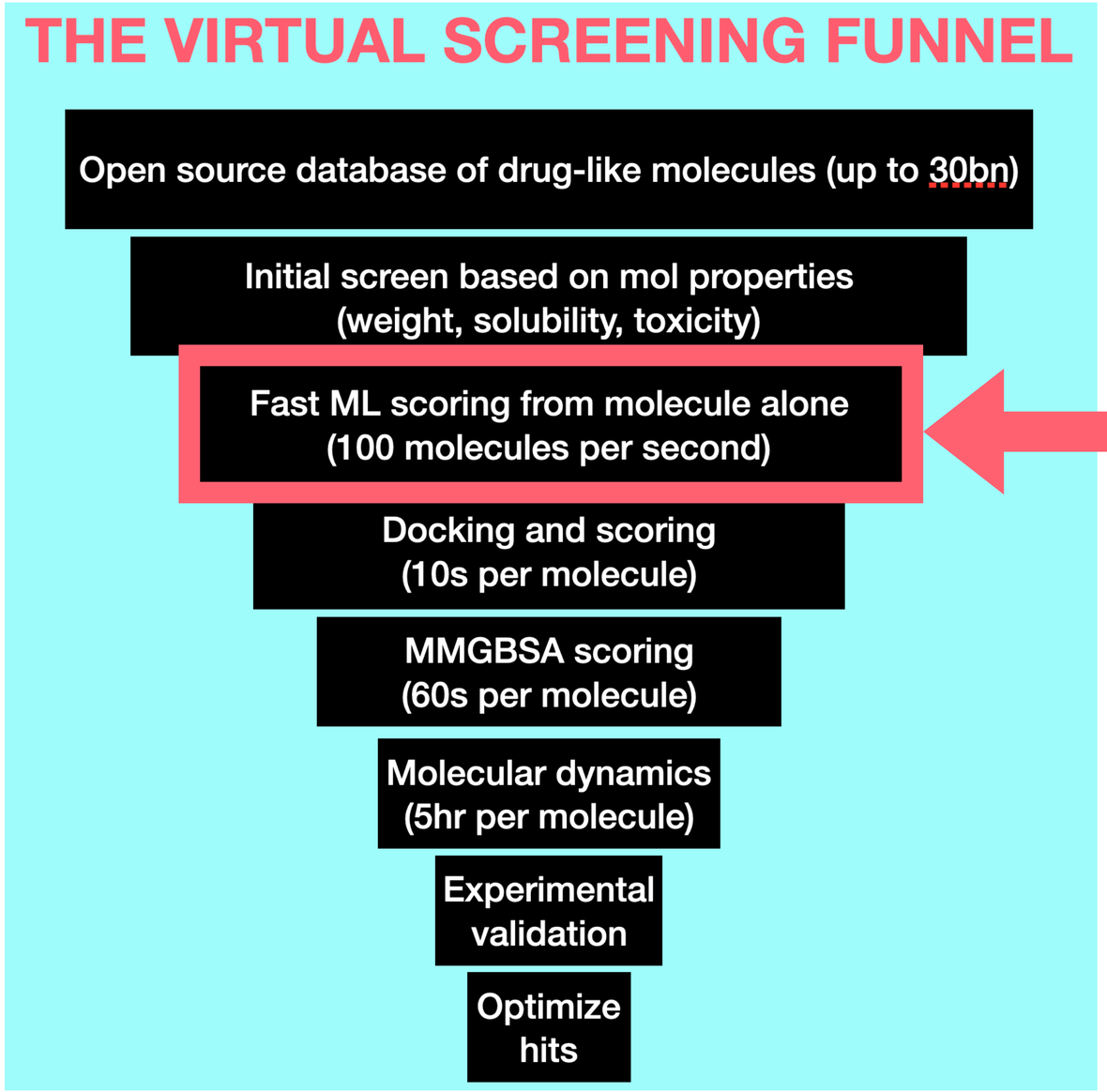
4. Lab tests

5. Animal trials

6. Human trials

Akshay Sethia, Alice Cheng, Ferdie Krammer, Gbetondji Dovonon, Jude Wells

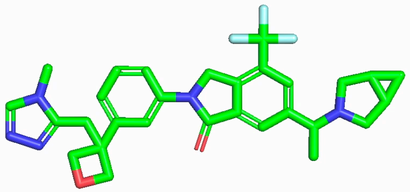
our approach

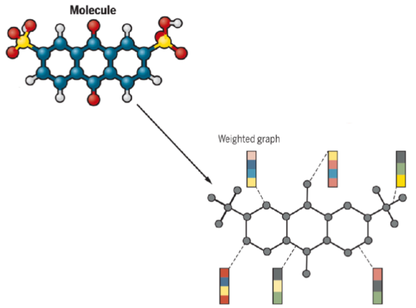


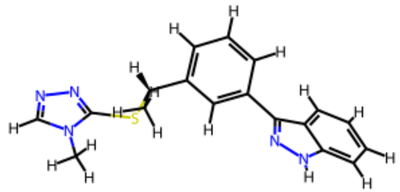
Binary classification experimentally observed hits vs. decoy molecules

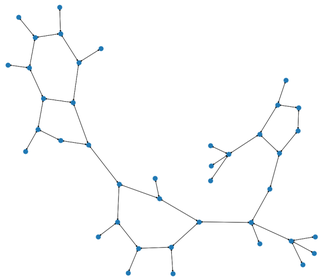
Molecules as graphs + GNNs

- Message passing graph neural networks
- Graph classification: one graph per molecule
- Atoms are nodes
- Chemical bonds are edges



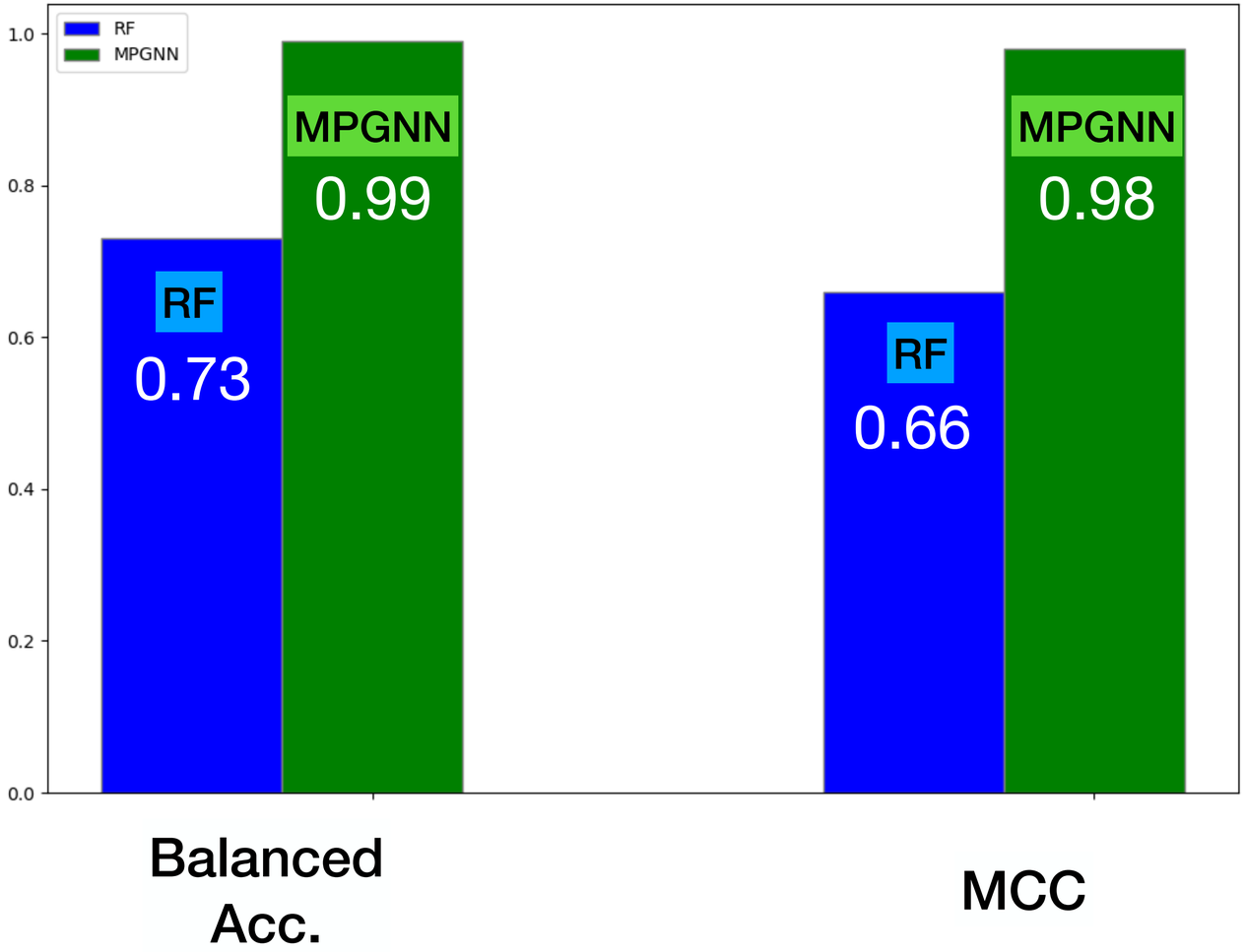


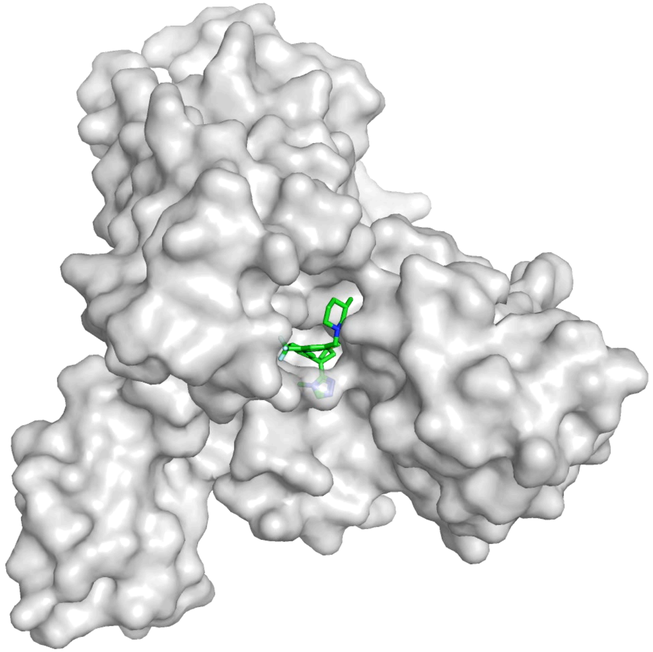




results: message passing GNN vs RF

GNN doing suspiciously well





Future directions

- Develop custom graph embeddings for molecules
- Bayesian optimisation loop with ML + physics based scoring
- Transfer learning from other protein-ligand pairs