



**What is virtual screening and why is it used?**

- Virtual screening
  - use of computation to estimate the activity (e.g. binding or inhibition) of a database of chemical compounds against a target
  - “virtual” in contrast to experimental high-throughput screening (HTS)
  - usually based on molecular docking, but machine learning in vogue

- Why is it used?
  - to help obtain leads for drugs and chemical probes
    - prioritizing compounds for experimental follow-up
    - faster predictions of specificity
  - compared to HTS
    - cheaper, accessible to academic laboratories
    - can screen larger libraries, increasing likelihood of good hit
    - HTS suffers from pan-assay interference compounds (PAINS)



# What is virtual screening and why is it used?

- Virtual screening
  - use of computation to estimate the activity (e.g. binding or inhibition) of a database of chemical compounds against a target
  - “virtual” in contrast to experimental high-throughput screening (HTS)
  - usually based on molecular docking, but machine learning in vogue
- Why is it used?
  - to help obtain leads for drugs and chemical probes
    - prioritizing compounds for experimental follow-up
    - faster predictions of specificity
  - compared to HTS
    - cheaper, accessible to academic laboratories
    - can screen larger libraries, increasing likelihood of good hit
    - HTS suffers from pan-assay interference compounds (PAINS)

## Single Docking

## Library Screen

Use GUI

Use scripts

Data in one directory

Data in tree structure

Single ligand PDBQT

Several ligand PDBQT

One interactive calculation

Submit jobs to cluster

Visually inspect all results

Visually inspect best results