What is virtual screening and why is it used?

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  - 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
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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

based on Morris et al, 2008