



**What is a virtual screening hit and what are some desirable properties of a hit?**

• Virtual screening hit has a good binding score

- If there is a positive control, the docking score is comparable or lower than the positive control

- Ideally, a virtual screening hit should
  - have a number of clear contacts with the receptor
  - have most atoms in contact with the receptor, opposed to in solvent



# What is a virtual screening hit and what are some desirable properties of a hit?

- A virtual screening hit has a low docking score
- If there is a positive control, the docking score is comparable or lower than the positive control
- Ideally, a virtual screening hit should
  - have a number of clear contacts with the receptor
  - have most atoms in contact with the receptor, opposed to in solvent

# How are virtual screening program assessed?