

# 2/27/2020 Week 7 Module 2

## Virtual screening

- This module will consist of
  - an introduction to virtual screening
  - a “tour” of a virtual screening calculation using AutoDock Vina on XSEDE Bridges
- At the end of this module, you should be able to answer the following questions:
  - What is virtual screening and why is it used?
  - What types of chemical libraries are used in virtual screening?
  - How is a chemical library prepared for virtual screening?
  - What is a virtual screening hit and what are some desirable properties of a hit?
  - How are virtual screening programs assessed?
- After the tour, you are encouraged to set up a virtual screening calculation with your own target

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