

2/27/2020 Week 7 Module 2

Virtual screening + MD in explicit solvent

- This module will consist of
 - an introduction to virtual screening
 - a “tour” of
 - a virtual screening calculation using AutoDock Vina on XSEDE Bridges
 - an explicit solvent MD simulation using OpenMM 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?