2/20/2020 Week 6 Module 2
Introduction to Molecular Docking

- This module will consist of
  - a lecture on molecular docking
  - an interactive exercise on molecular docking with AutoDock
- At the end of this module, you should be able to address these questions:
  - What is molecular docking?
  - What is it good for?
  - How does it work?
  - What are its key approximations?

What is molecular docking?

- To predict
  - the 3D structure of a noncovalent complex
    - protein-ligand
    - protein-protein
  - the binding affinity of the partners (scoring)
- Prior to prediction, structure of binding partner(s) may be known, but
  - could be affected by binding
  - may be bound to different partners