2/25/2020 Week 7 Module 1
Molecular docking with AutoDock Vina

- This module will be a tutorial on AutoDock Vina
  - docking program developed at The Scripps Research Institute
  - http://vina.scripps.edu
- After this module, you should be able to set up and run a molecular docking calculation using AutoDock Tools and AutoDock Vina

Why AutoDock Vina?

- There are many molecular docking programs
- Why AutoDock Vina?
  - Free
  - Works on multiple platforms
  - Fast
  - Very popular
    - >10,000 citations of primary reference [Trott and Olson, 2010]
    - >1,400 citations to primary reference of AutoDock 3 & 4 [Morris et al, 1998]
  - Available on XSEDE bridges
  - AutoDock Tools GUI