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

Comparison of AutoDock Versions

AutoDock 4	AutoDock Vina
	2 orders of magnitude faster. Parallelized code.
Lennard-Jones sterics	Gaussian sterics
Lamarkian genetic algorithm	Gradient-based optimizer
Pre-calculated grid maps	On-the-fly grid maps

Today's Tutorial

- Using AutoDock 4 with AutoDock Tools (http://autodock.scripps.edu/faqs-help/tutorial/using-autodock-4-with-autodocktools)
  - Download the input files
  - Read the instructions
- Do the following exercises
  - 1
  - 2: pay attention to the torsions
  - 3: pay attention to the grid in relation to the binding site
  - 4
  - Skip 5-7, which are specific to AutoDock 4
  - 2nd half of 8
  - 9 is optional
  - 10

References

- Morris, G. M.; Goodsell, D. S.; Halliday, R. S.; Huey, R.; Hart, W. E.; Belew, R. K.; Olson, A. J. Automated Docking Using a Lamarckian Genetic Algorithm and an Empirical Binding Free Energy Function. Journal of Computational Chemistry 1998, 19 (14), 1639–1662.
- Trott, O.; Olson, A. J. AutoDock Vina: Improving the Speed and Accuracy of Docking with a New Scoring Function, Efficient Optimization and Multithreading. Journal of Computational Chemistry 2010, 31 (2), 455–461.