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