

# Comparison of AutoDock Versions

AutoDock 4	AutoDock Vina
	2 orders of magnitude faster. Parallelized code.
Lennard-Jones sterics	Gaussian sterics
Lamarckian 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