

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.