

# Exercise 5

Molecular Statistic, Week 5

2014

## 1 Introduction

Writing simulations is one thing, but sometimes it is also necessary to data-mine, manipulate and visualize data. Python is great for this, and so the goals of this exercise is:

1. Use Python to load/read data
2. Use numpy to manipulate data
3. Use matplotlib/pylab to illustrate
4. Save Numpy data

## 2 Exercises

Which will be done with small individual exercises.

### 2.1 Dissociation energy of a water dimer

1. Convert the distance from A.U. to Ångstroem.
2. Convert the energy to kJoule/mol. Plot the result
3. Convert the energy to kcal/mol. Plot the result.