

Linux Self-Test

Purpose: Beyond the simple basics of unix, there are certain tasks that you should be comfortable doing, as they are representative of the sort of meta-work that computational chemists and structural biologists do on a routine basis. These include finding and editing files, translating file formats, comparing file contents, extracting data from files, and converting the output of one program into the proper format for input into another program. If any of the following tasks are difficult for you, you should spend time studying basic unix tools until they are easy for you.

1. Examine the directory /home/momokurs/rosetta_workshop/
 1. How much disk space is used by the files and subdirectories?
 2. Which subdirectory takes up the most space?
2. Imagine that you have created a file somewhere under /home/momokurs/rosetta_workshop/ However, you don't remember its exact name- it's probably something similar to **4TQ5something.out** but you don't remember what the '**something**' is.
 1. How can you locate the file efficiently?
 2. Examining the file you found, the third line of the file will show the values of the Rosetta score terms for the first structure. How can you print out just the first three lines of the file? ("Print" to the screen, not to a printer.)
 3. This file contains a line that starts with "SCORE:" for each structure it contains. How many structures are in this file?
3. Download 1DMO.pdb to your working directory. (If you are not familiar with pdb.org, then you should explore it a little.)
 1. Is that the letter O or a zero? How could you tell?
 2. Use four different commands to examine the text inside the file.
 3. How many lines in the file start with 'ATOM'?
 1. Repeat this with another tool (e.g. if you used **grep** the first time, use **awk** this time.)
 4. What column number contains the chain ID? (Hint: use **cut -c**) Does **awk** agree?
 5. Extract the first model from the NMR ensemble and save it as my_model.pdb
 6. Compare it to the example file one_model.pdb. Exactly how does it differ? Are the differences significant?
4. Read the manual page for bash. You don't need to read the whole thing, but get familiar with the sections, and explore questions such as:
 1. How can you repeat the previous command without typing it?
 2. How can you repeat the previous command with one word changed?
 3. How can you apply a command to many files consecutively?
5. Removing spaces from filenames:
 1. Perform the example in filenames_with_spaces/
 2. Search the web for an alternative method. Why would it be better or worse than the example given?