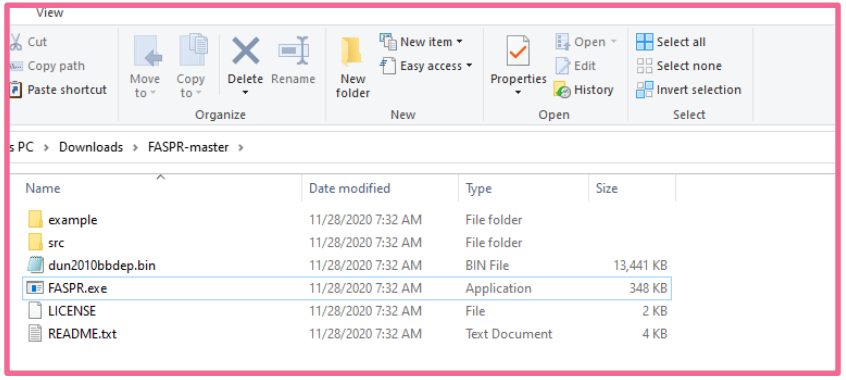
THIS INSTRUCTION APPLIES TO WINDOWS SUBSYSTEM FOR LINUX

i

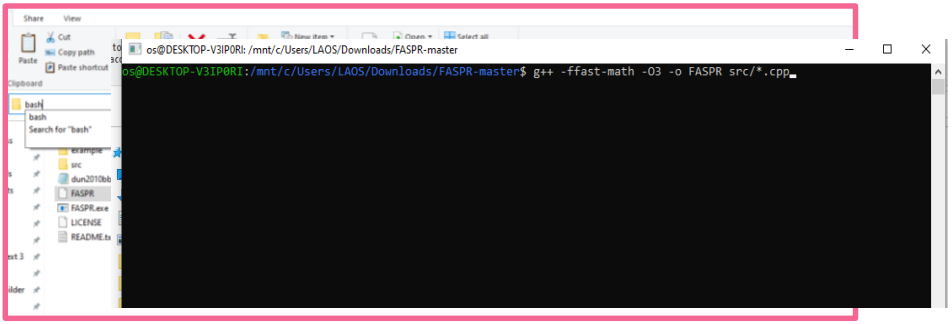
Download FASPR from https://github.com/tommyhuangthu/FASPR and extract to any folder as below. Then enter/open the folder



ii

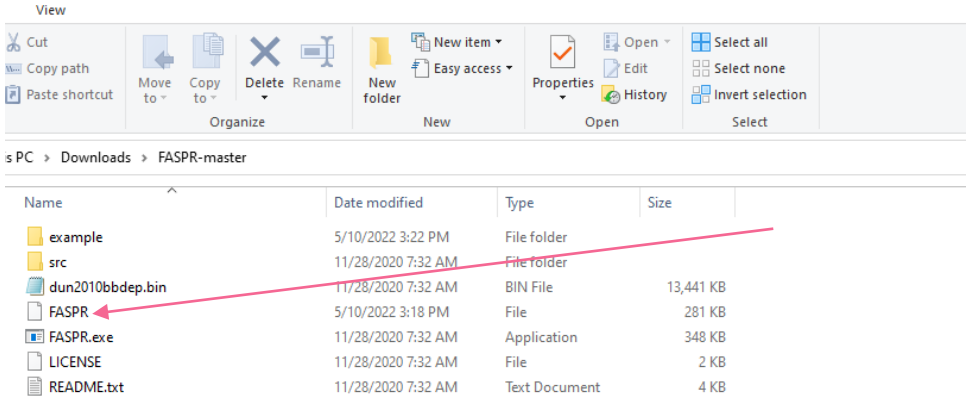
Type “bash” in the search window and hit enter to open lunix terminal as shown. Then, execute the code below to compile FASPR (it takes ≈ 1 min to compile):

g++ -ffast-math -O3 -o FASPR src/*.cpp



iii

After successful compilation you will see FASPR as pointed towards



iv

Now install PRAS server (if not installed). Note that **linux_examply.py** is in the folder containing this document. **If copying the last code below will lead to error, use the one provided in syntax.txt**

Install PRAS server which is added to path automatically with:

pip install Pras-Server==1.0.5

Now download 1aho.pdb and copy to the current folder and run the following code to repair several missing atoms using chi from FASPR PDB output

./FASPR –i 1aho.pdb -o out.pdb;python3 linux_example.py 1aho.pdb “” “” out.pdb

This is not a substitute for FASPR installation instructions. Always refer to the software documentation