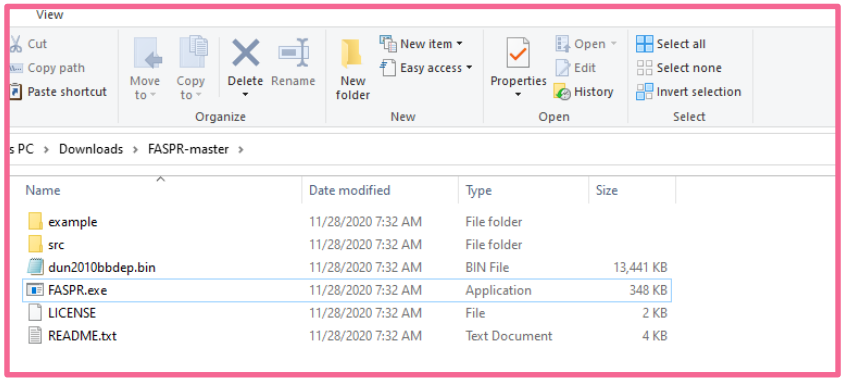
THIS INSTRUCTION APPLIES TO WINDOWS SUBSYSTEM FOR LINUX

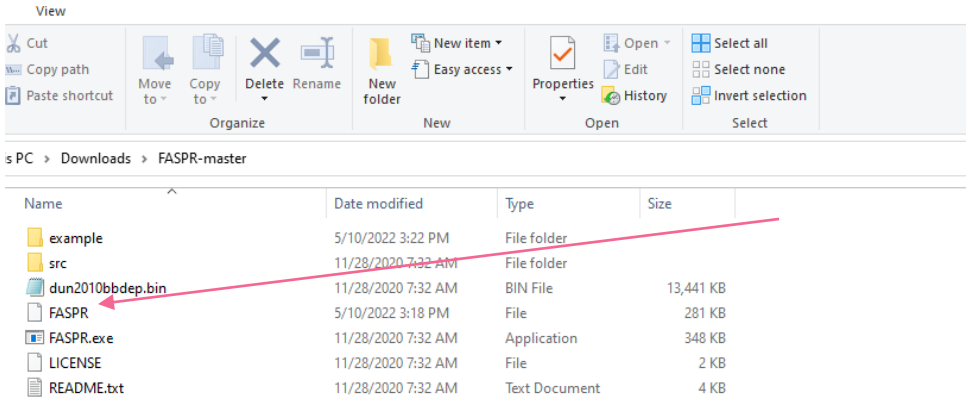
i

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



iii

After successful compilation you will see FASPR as pointed towards

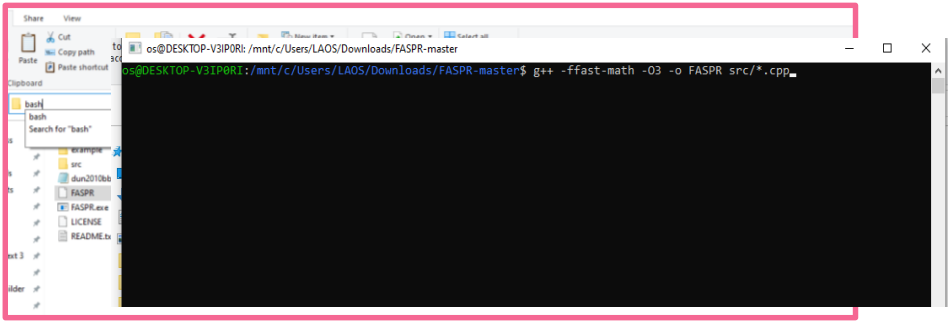


There seems to be a bug in the current version of FASPR, so open src/FASPR.cpp:
In line 72, change string pdbin=(string)"example/1mol.pdb" to string pdbin=(string)“.“
In line 73, change string pdbout=(string)"example/1mol_FASPR.pdb" to string pdbout=(string)“.“
Without these changes, your input PDB and its path must correspond to example/1mol.pdb

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



iv

Now install PRAS server (if not installed) using the command below

Install PRAS server which is added to path automatically with:

pip install Pras-Server==1.0.10

Now download 1aho.pdb and copy to the current folder and run the code in **syntax.txt** that invokes **linux_examply.py** in the folder containing this document to repair several missing atoms using chi from FASPR PDB output.
It is a good practice to type commands in Linux than copy and paste as Linux is extremely sensitive.

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