Commands Entered in the terminal

1. Open a terminal.
   - Linux users press **Ctrl**, **Alt** and **T** keys together.
   - **Ubuntu** 20.04 app for **Windows** users.
2. Change to **Documents** folder
   - Linux users can type cd **Documents** and press the **Enter** key.
   - Windows users need to enter an extra command to create the **Documents** folder first.
   - Type, **mkdir Documents** and press **Enter**.
   - Then, type **cd Documents** and press **Enter**.
3. Press **Enter** to execute a command in the **terminal**. Further on this will not be mentioned separately.
4. Create a new working directory to store all the files.
   - Enter the command, **mkdir firstmd**.
5. Change to the working directory.
   - Enter the command, **cd firstmd**.
6. Windows users must find the path of this directory assigned by your **Windows OS**. Detailed instruction is provided in the next section.
7. Then copy the provided input file, **1AKI.pdb** to this directory.
   - Windows users can use file manager to copy and paste the file.
8. Enter the command **gmx pdb2gmx -f 1AKI.pdb -o first.gro**
   - Type, 4 at the prompt to select **AMBER99** and press **Enter**.
   - Then type 2 at the prompt to select **Tip4p** option and press **Enter**.
9. Enter the command **gmx editconf -f first.gro -o box-added.gro -c -d 1 -bt cubic**

Finding path of user files created via Ubuntu 20.04 app in Windows 10 OS

Section 1

1. Create a folder **firstmd** as mentioned in the previous page.

Section 2

1. Open the file explorer.

2. First show the hidden files and folders in the system.

   - For this click on **View**, **Options**, change folder and search options.
   - In the dialog box, select the **View** tab.
   - Click on **Advanced settings**
   - Check the box for **Show hidden files, folders and drives**.
   - Click on **Ok**.

> *Make sure not to delete, modify or move system files of Windows.*
>
> *They are hidden to prevent accidental changes from the user to protect your windows 10 OS.*

3. Select **C** drive from the left panel, where **Windows 10 OS** is installed.

4. Type, **firstmd** in the search form on the top right to search for the path and press **Enter**.

5. Wait for the search results. This may take some time, depending on your computer.

6. Note down the path carefully and remember it for future use.

7. The **..** seen on display means, it is too long to display and there is data inside it.

8. Make sure to note down the full path.

9. Navigate to this directory and notice the firstmd folder that you created using **Ubuntu app**.

10. This path is the home directory for **Ubuntu 20.04 app**.

11. The path that you see here is the path in **Windows 10 OS**.

12. After the **MD** run, the results will the stored in this path.

13. You will need to access the files stored/saved in this path in **Windows 10 OS**.

Section 3

1. You may also save files in this path in **Windows 10 OS**.

2. They are accessible from the terminal in **Ubuntu 20.04 app**.

3. However, to read or edit them via **Ubuntu 20.04 OS**, you will need to change the permission via **terminal** commands.

4. Use the command **chmod 770 filename/directory-name** to make the file readable and editable.

5. Use the command **chmod 777 filename/directory-name** to make the file read, write and executable.