

VSpice – GUI Installation Guide for Windows

Accessing and downloading VSpice-GUI repository

- Access the GitHub repository
- Clone or go to the path or Executables/Windows/, and download the repo containing following files
 - *vspice-gui-windows-app.exe* (executable file and can be run either through terminal or directly by double clicking on the app)
 - *vspice-tools/* (directory containing all required files to run vspice-gui-windows-app.exe application)
- Clone or download *vspice-libraries.zip* file. It contains already minimized libraries provided by vspice-gui

Installation of dependencies needed to run VSpice-GUI

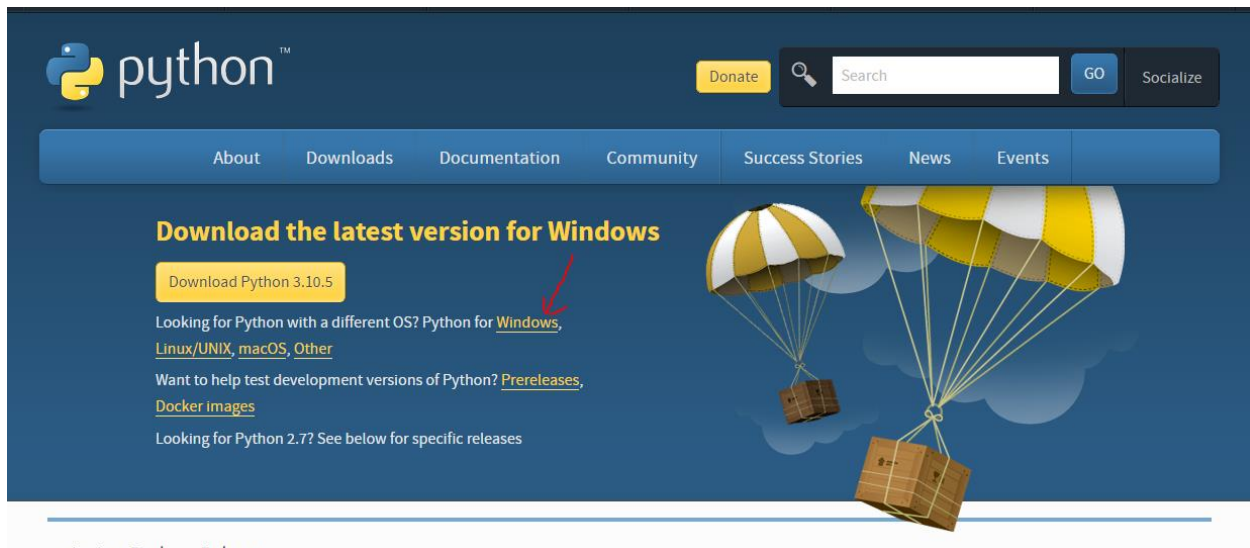
1. **Python latest version** (mandatory for running vspice-gui)
2. **Python2.7** (mandatory for running vspice-gui)
3. **MGL Tools** (required for receptor preparation and compounds library preparation modules)
4. **Open Babel** (required for compounds library preparation modules)
5. **Rscript** (required for filtration module)

Please note if you do not need to run particular modules, you are not needed to install all the dependencies, and you may skip the modules' dependencies that you are not running. For example, if you do not need to filter the result of screening then you may skip installing R. However, it is strongly recommended that you should install all the modules listed above to utilize the full functionality of the tool.

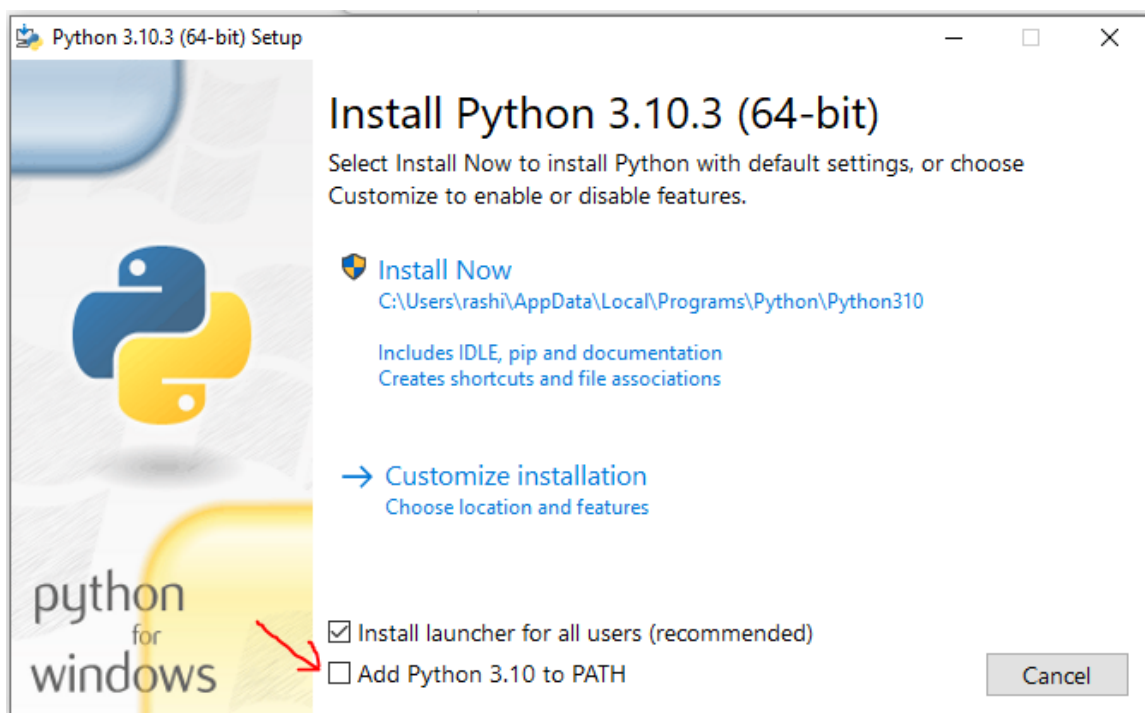
Note: You need to have administrative privileges to install vspice-gui

Python (latest version) Installation

1. Go to the URL <https://www.python.org/downloads/>
2. Please note that the currently updated version of python is 3.10.5, you may download the updated version depending on its release at the time of download. Click on windows as shown in the figure



3. Download windows installer of python
4. Install python as shown below

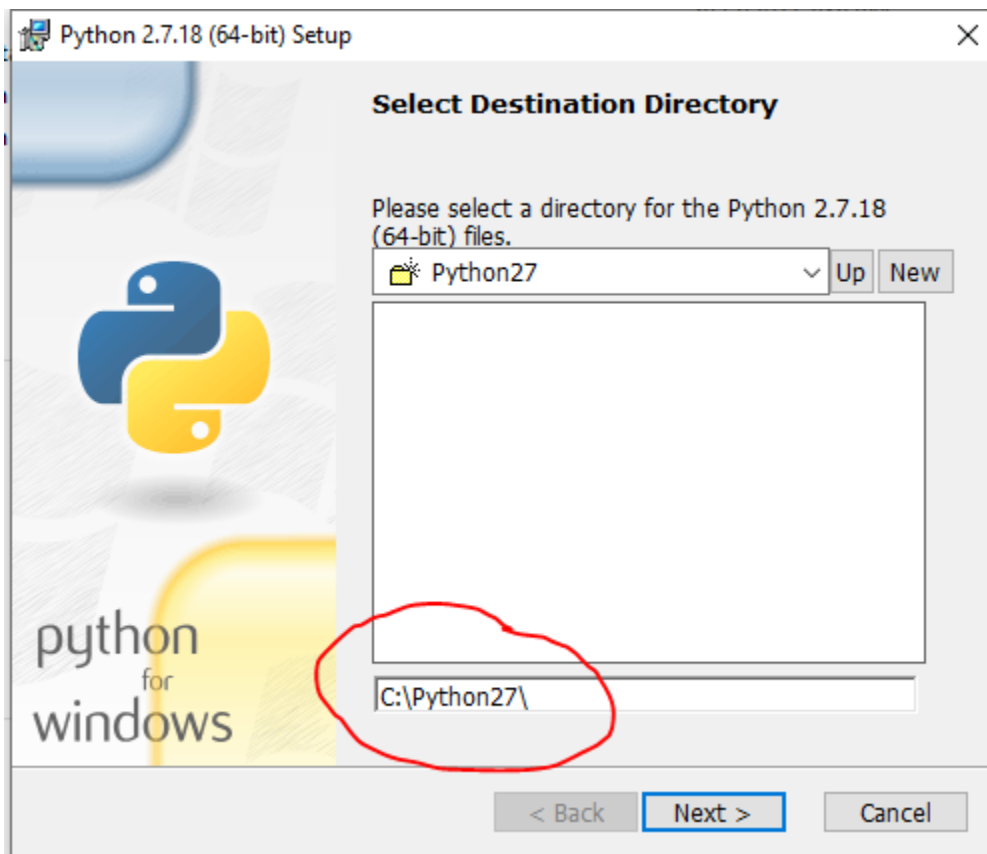
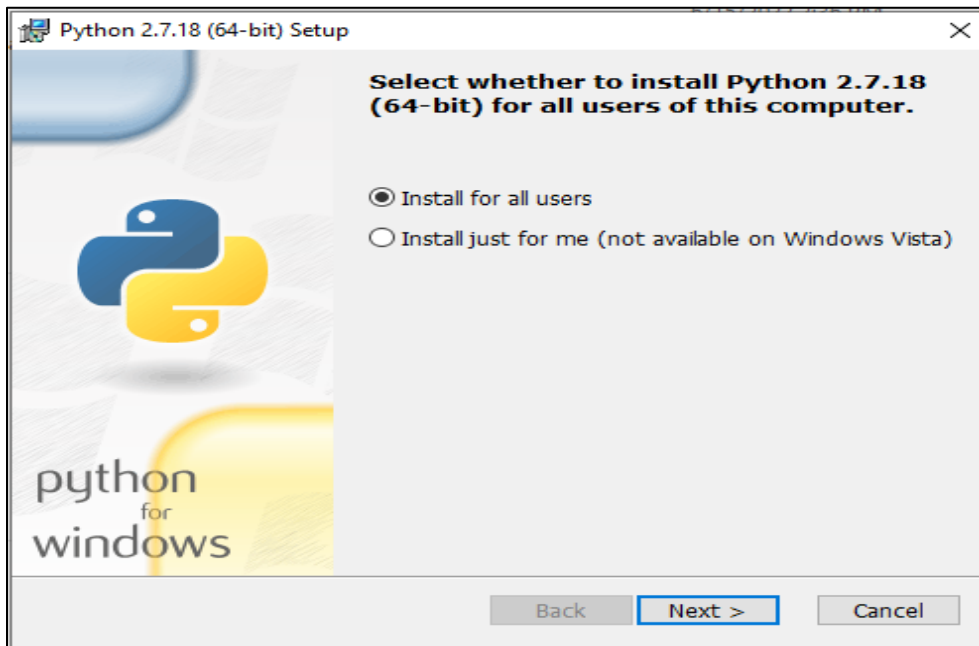


5. Make sure to check on the option as shown in the figure above
6. Click on the install now option
7. It will get installed

Python (2.7 version) Installation

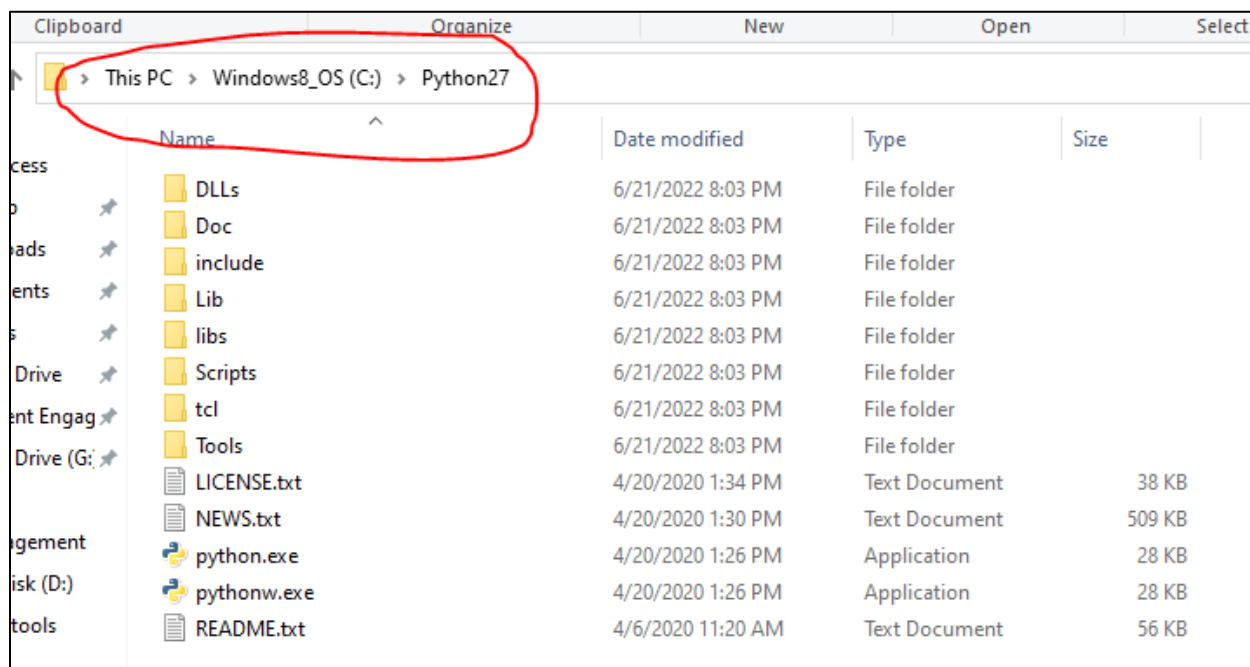
1. Go to the URL <https://www.python.org/downloads/>

2. Locate python version 2.7, and download it in your local disk
3. Click on installer for installation as shown below








Note the path for installing python 2.7

- Next choose the default option to install python.
- The path of recently installed python 2.7 is as shown in figure below (**C:\Python27**)

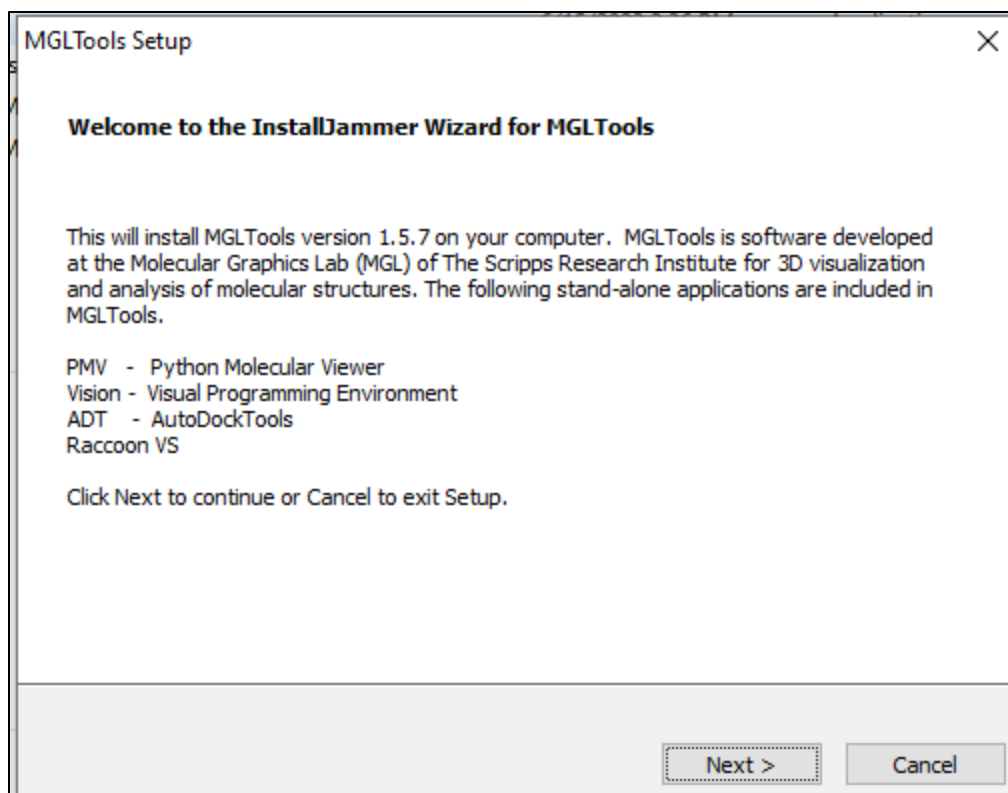


MGL Tool Installation

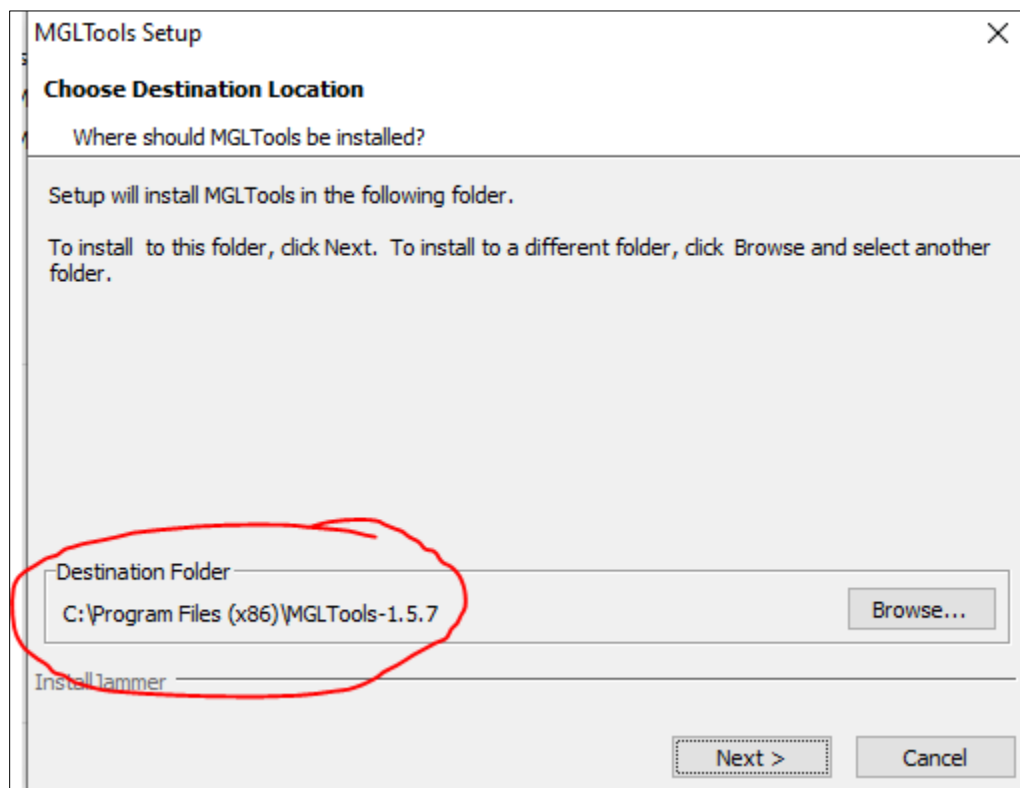
- Go to the link <https://ccsb.scripps.edu/mgltools/downloads/>
- Download the installer as shown below

| platform | installer |
|---|---|
|  | mgltools_win32_1.5.7_Setup.exe (80Mb) |
|  | mgltools-1.5.7-MacOS-X-Install.dmg (GUI installer 91Mb) |
|  | mgltools_1.5.7_MacOS-X.tar.gz (tarball installer 85Mb) |
|  | mgltools_Linux-x86_64_1.5.7_Install (Linux 64 GUI installer 109Mb) |
|  | mgltools_x86_64Linux2_1.5.7.tar.gz (Linux 64 tarball installer 108Mb) |

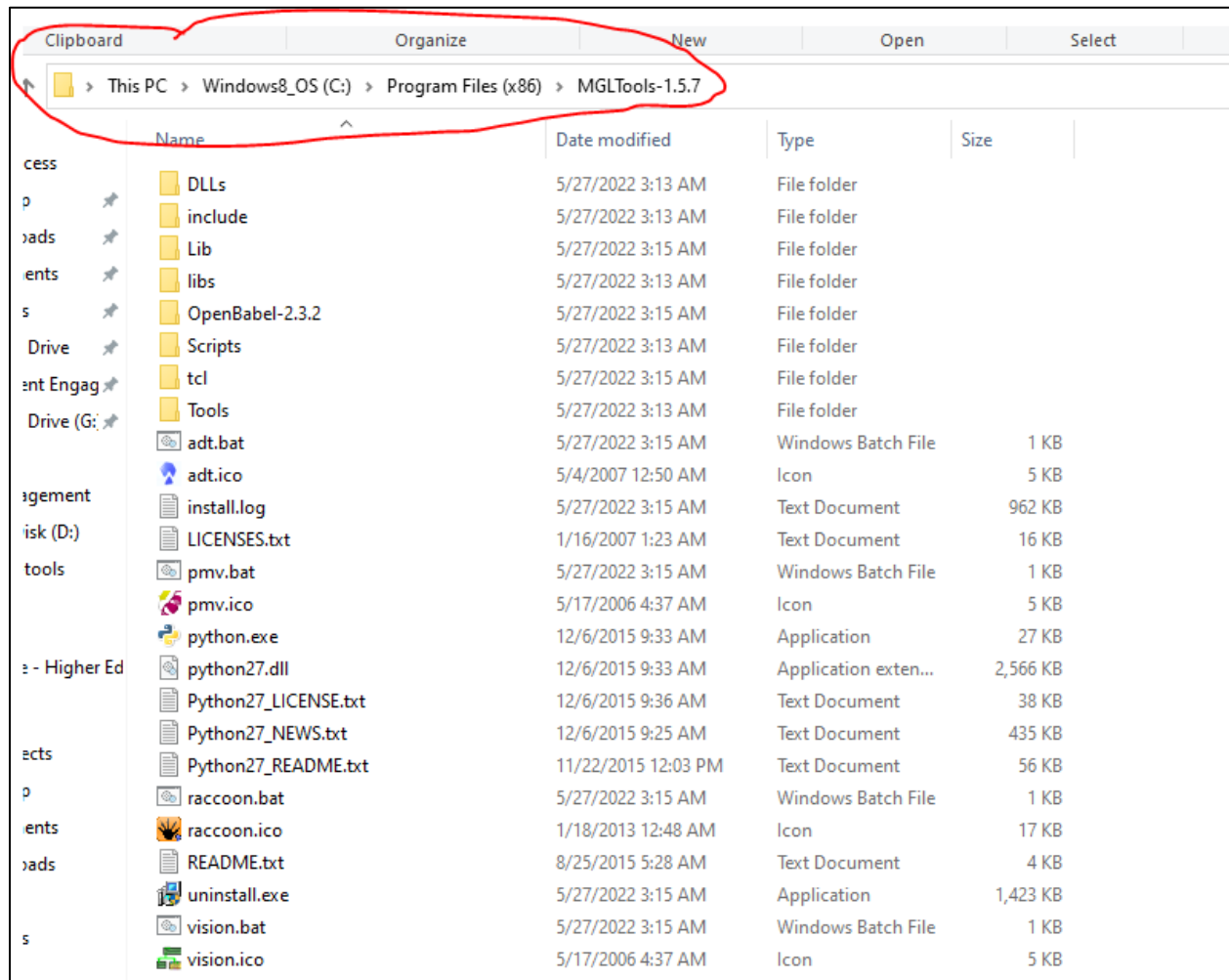
- Click on next



4. Note the path where mgl tools are going to install

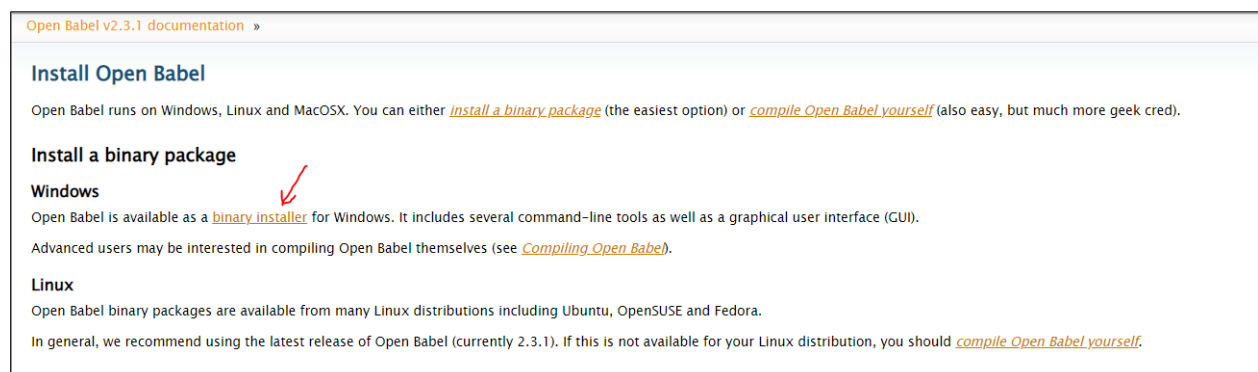


- By clicking next will install mgl tools in the desired location as shown below (C:\Program Files (x86)\MGLTools-1.5.7)

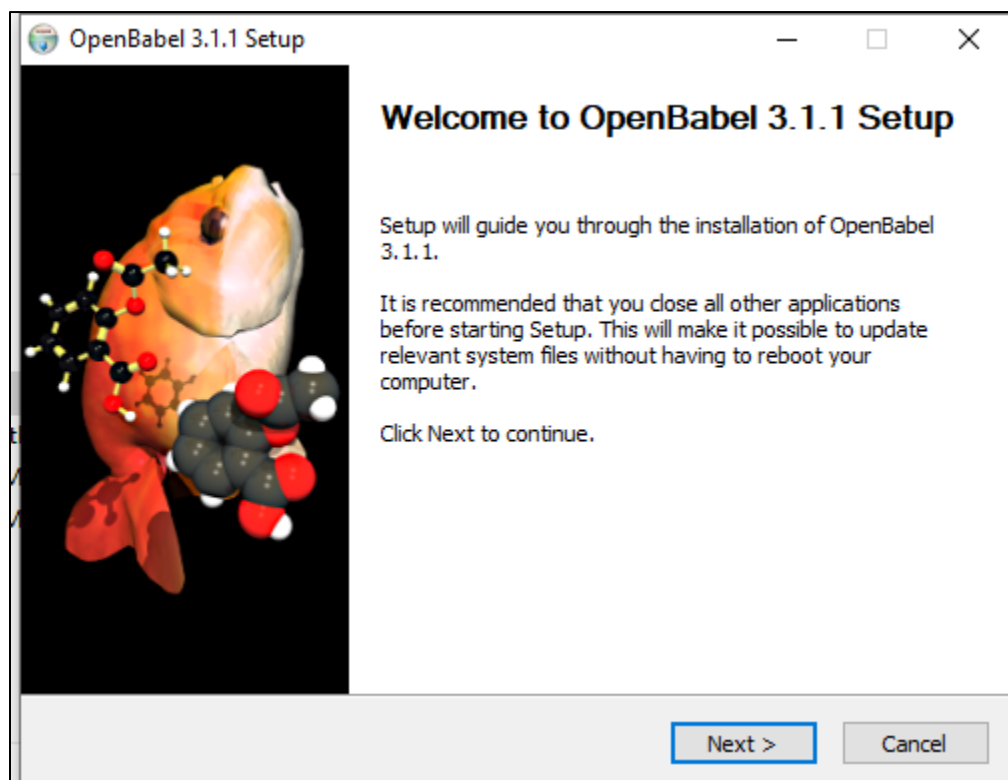


Open Babel Installation

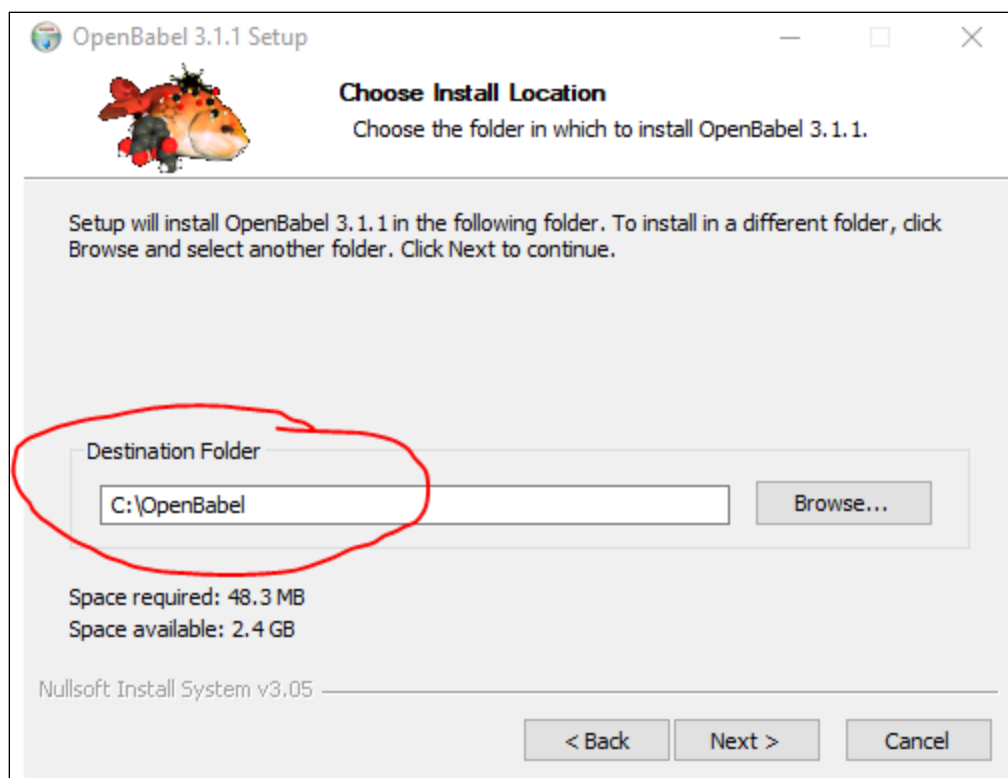
- Go to the link <https://openbabel.org/docs/dev/Installation/install.html>
- Click on binary installer as shown below



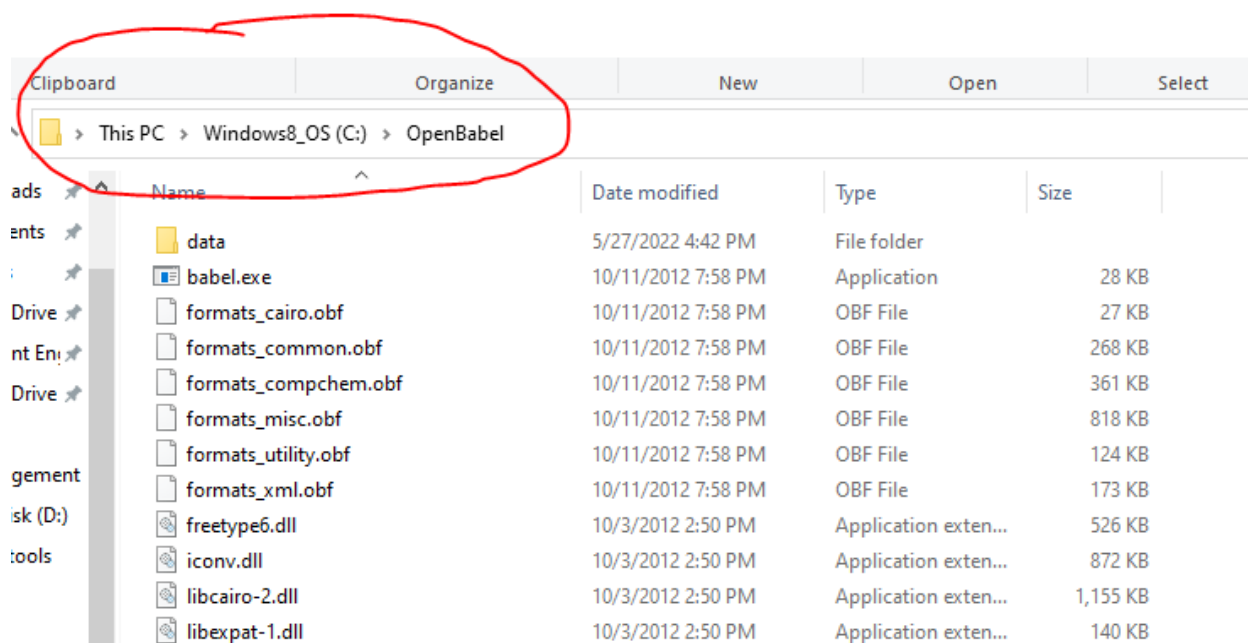
3. Click on installer to install open babel as shown below



4. Click on I agree
5. Change the installation path to (C:\ OpenBabel\)

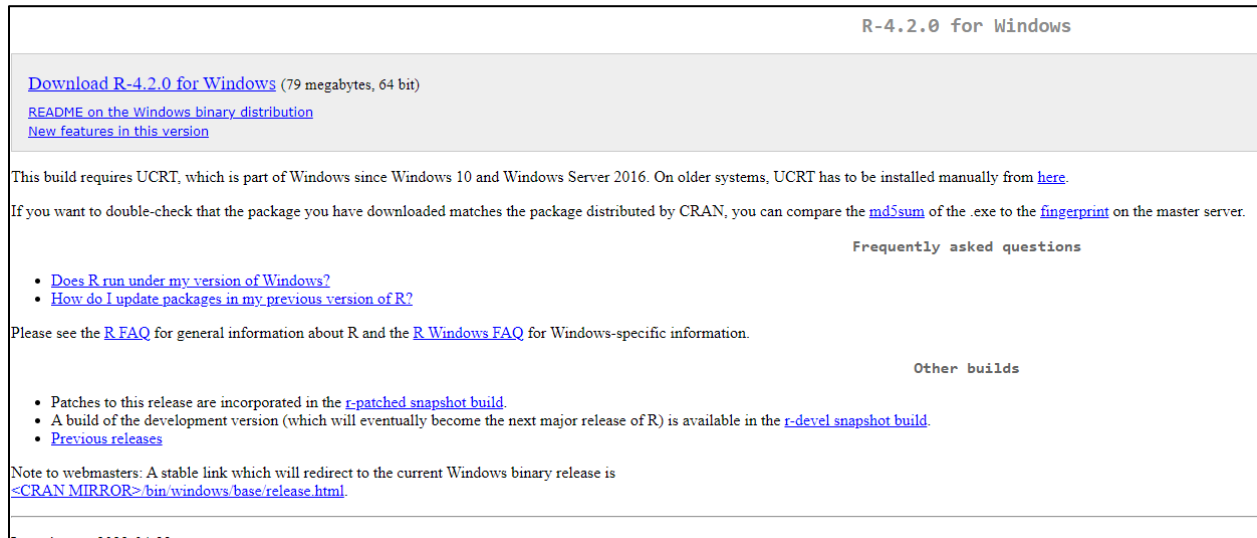


6. By clicking the next button will install Open Babel in the path as shown below
7. Make sure the installation path of Open Babel is [C:\OpenBabel](#)

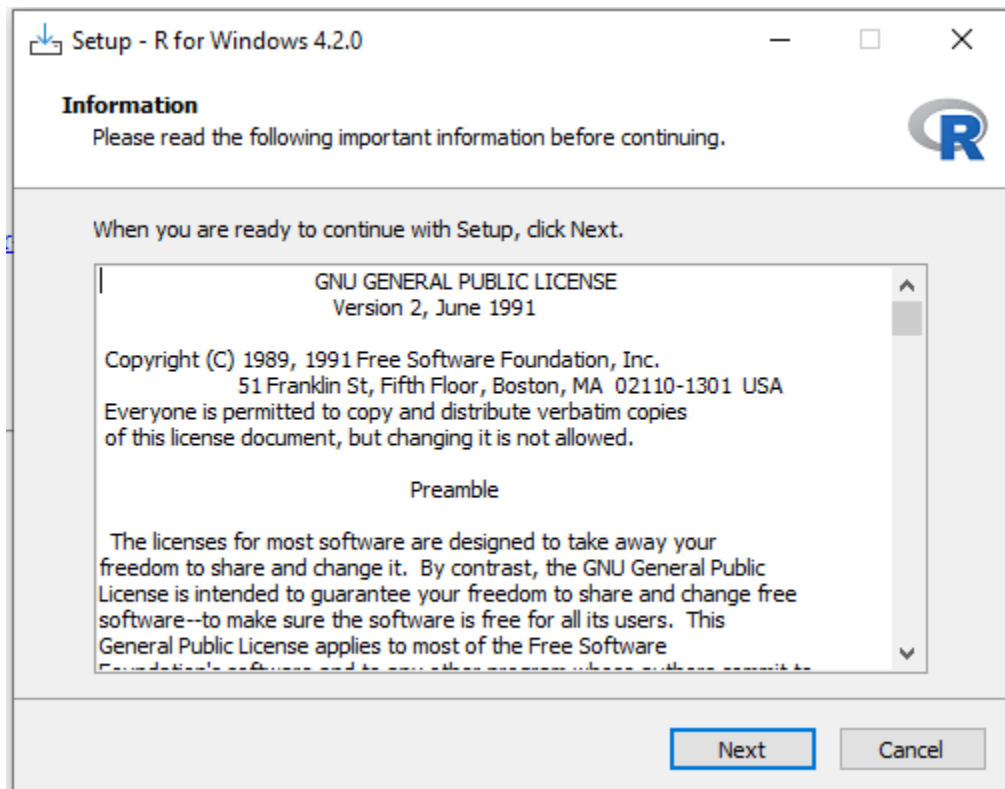


R Installation

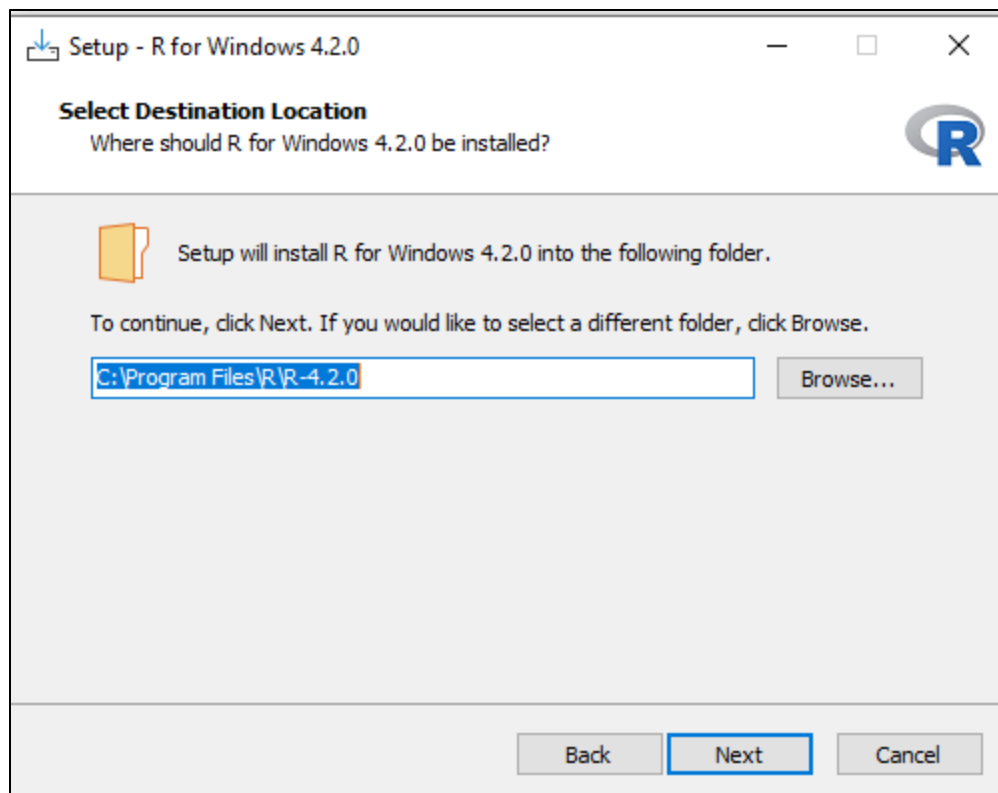
1. Go to the link <https://cran.r-project.org/bin/windows/base/>
2. Download the installer by clicking the download link as shown below



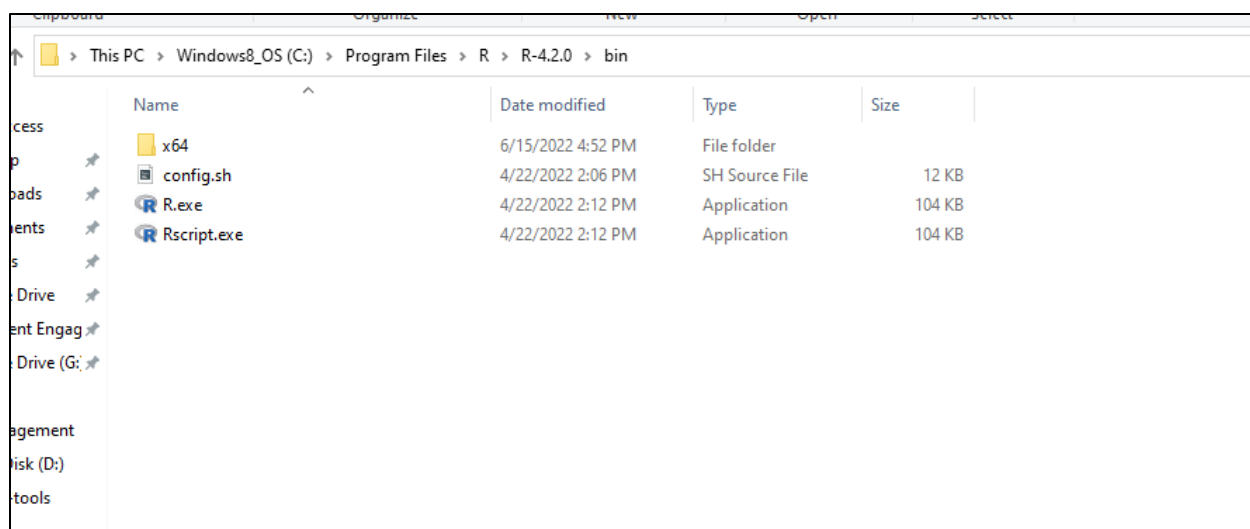
3. Click the installer to install R in your system as shown below



4. Note the path for installing R as shown below



5. By clicking next will install R in your system in the path (<C:\Program Files\R\R-4.2.0\bin>) as shown below



6. Copy this path into environmental variables as follows
 - a. Right click on the start menu and click on system
 - b. Click on advances system settings and click on environment variables as shown below

About

Your PC is monitored and protected.

See details in Windows Security

Device specifications

| | |
|---------------|---|
| Device name | Rashid-Lenovo |
| Processor | Intel(R) Core(TM) i7-5500U CPU @ 2.40GHz 2.39 GHz |
| Installed RAM | 8.00 GB |
| Device ID | 8324ECAB-A6DF-49C1-9244-7FC12C50FE43 |
| Product ID | 00326-10000-00000-AA583 |
| System type | 64-bit operating system, x64-based processor |
| Pen and touch | No pen or touch input is available for this display |

Copy

This page has a few new settings.

Some settings from Control Panel have moved here, and you can find your PC info so it's easier to share.


Related settings

[BitLocker settings](#)

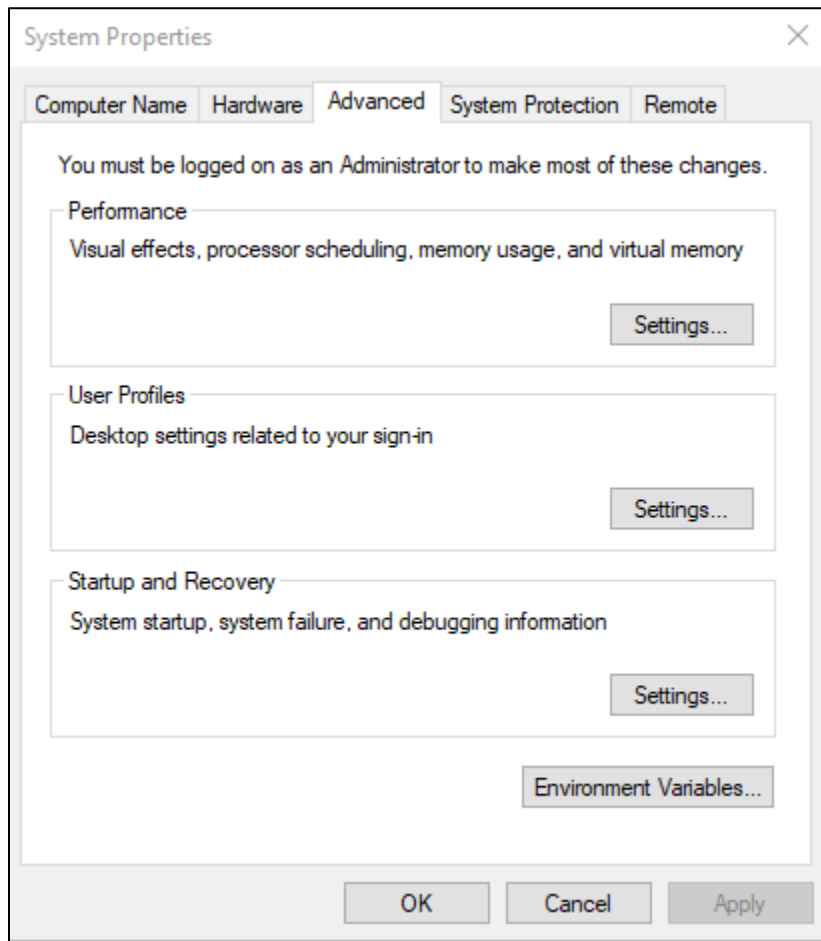
[Device Manager](#)

[Remote desktop](#)

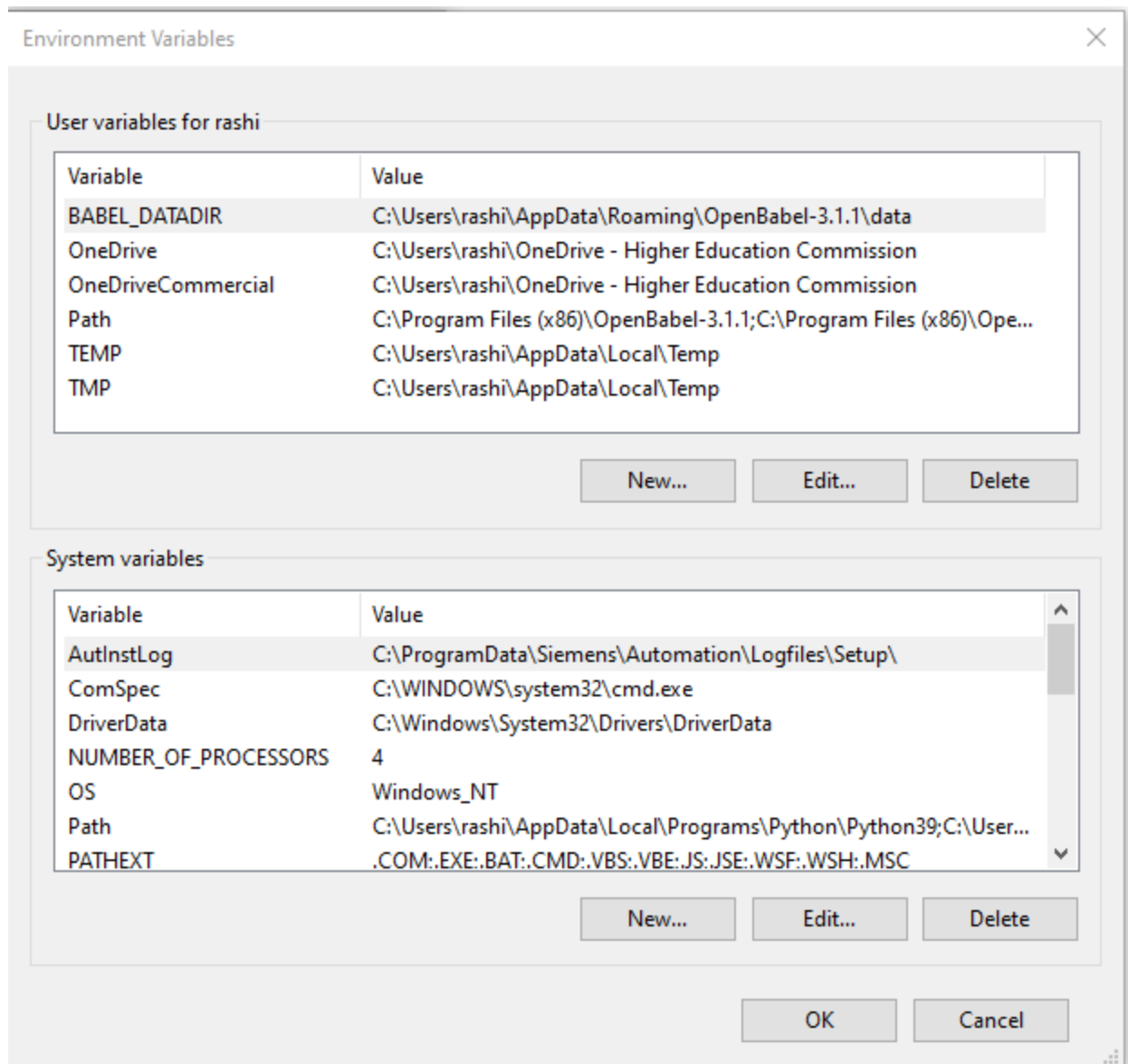
[System protection](#)

 [Advanced system settings](#)

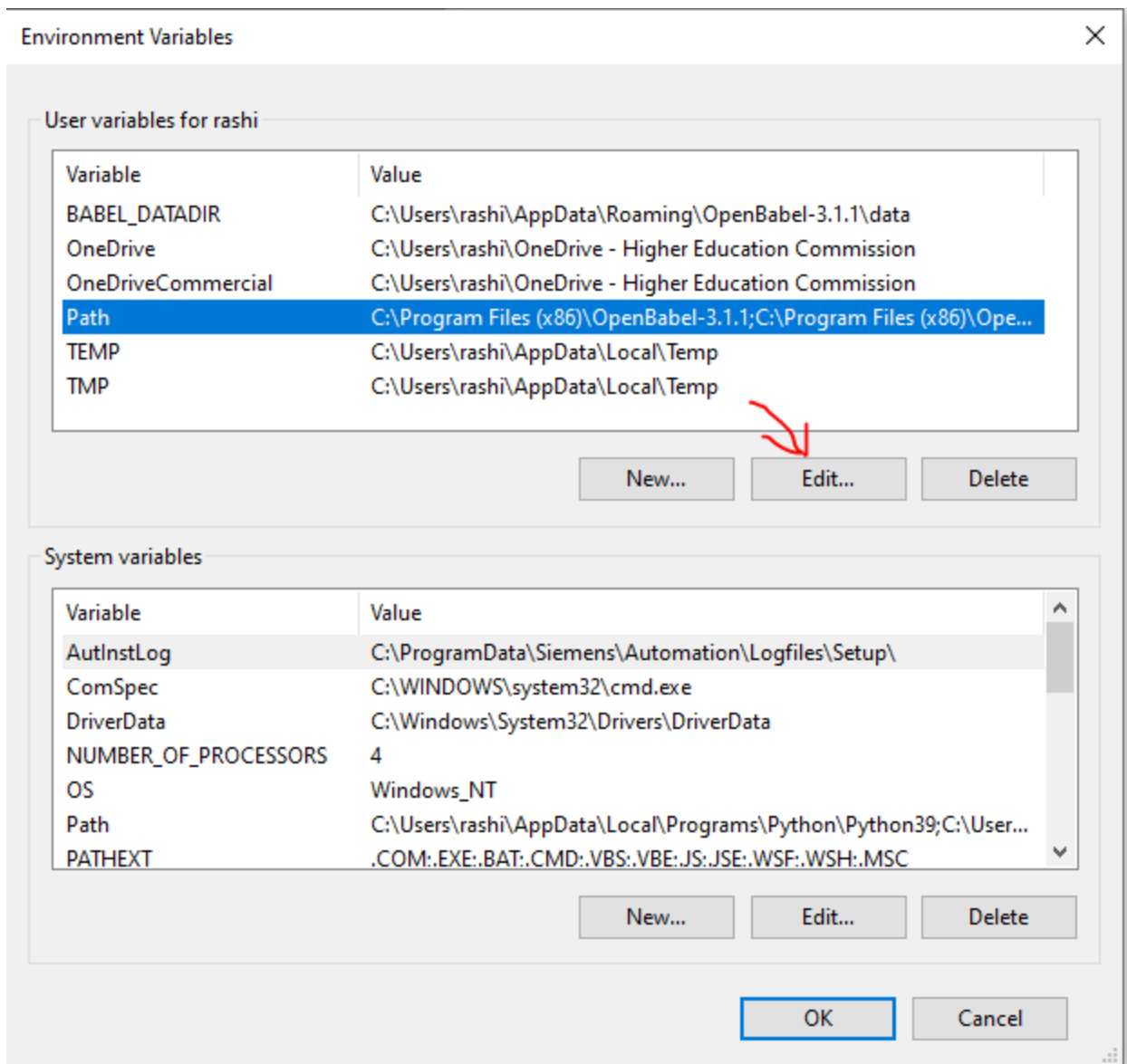
[Rename this PC \(advanced\)](#)



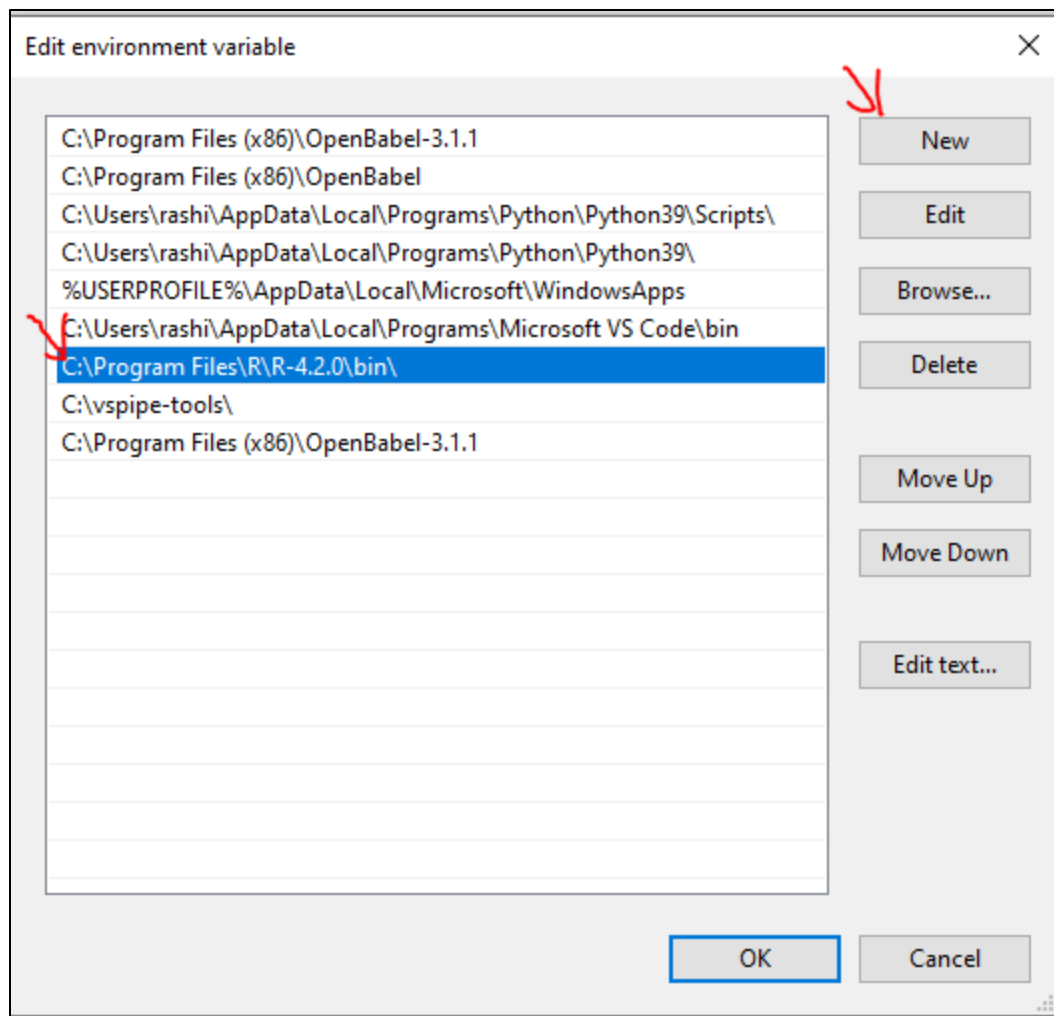
c. Click on path under User variables as shown below



d. Select path and click on edit



- e. Click on new and add the path as highlighted below



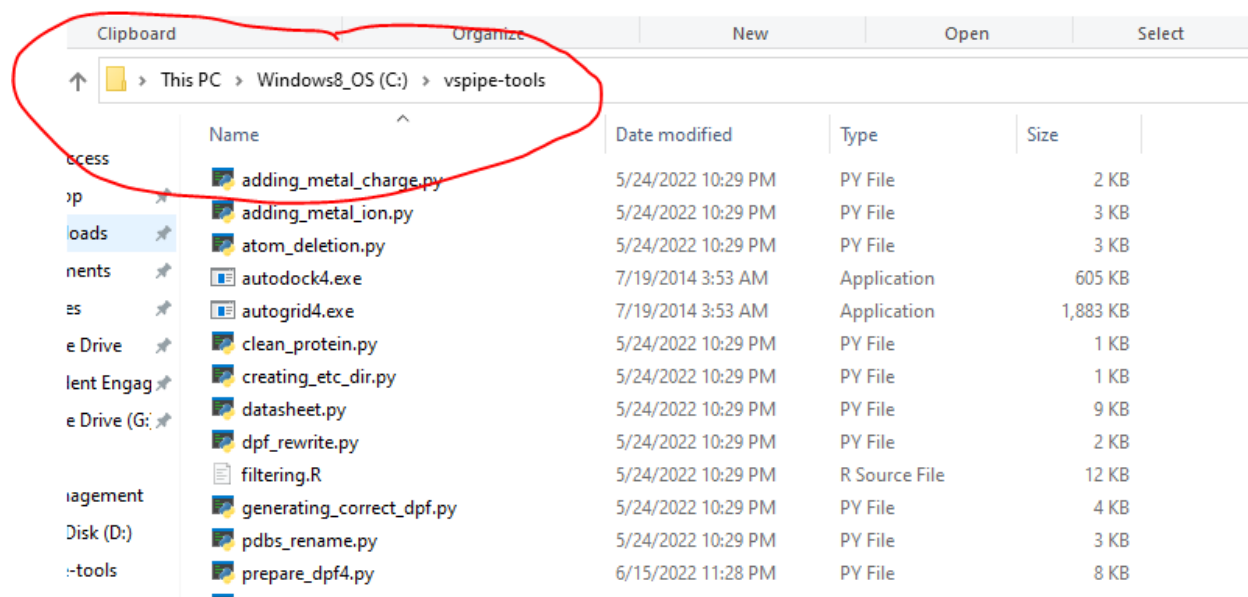
Getting files ready for running vspipe-gui

As stated earlier, the downloaded zipped folder, '**vspipe-gui-windows.zip**', must have following files/directories in it:

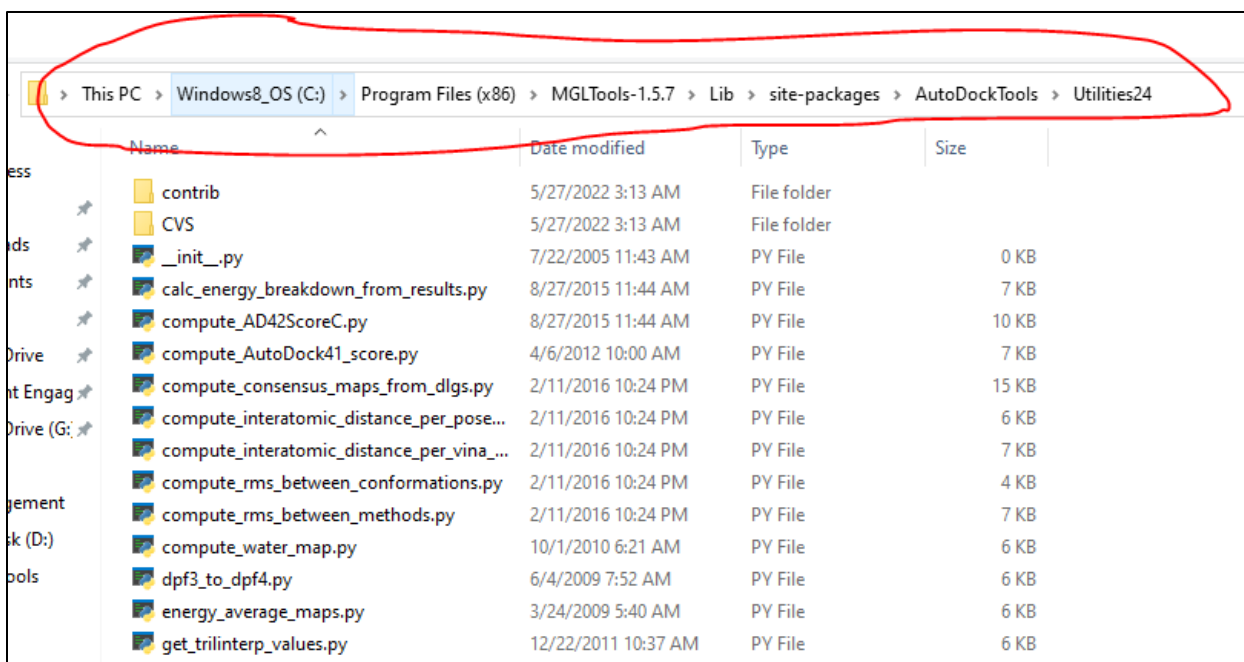
- vspipe-gui-app.exe
- vspipe-tools/
- vspipe-libraries.zip/

Following is the step-by-step guide to get files ready for running vspipe-gui successfully:

1. Unzip the folder, and copy vspipe-gui-app.exe file to the desktop in order to run vspipe-gui from the desktop.
2. Copy vspipe-tools folder to C drive as [C:\vspipe-tools](#)



3. Unzip vspipe-libraries.zip and copy the folder, '**minimised_libs**' to C drive as [C:\minimised libs](#)



- Copy this path and open the above-mentioned five files in **C:\vspipe-tools** path one by one in notepad or word pad.
- Replace the header line (yellow highlighted) with the path that you have copied as shown in figure

```

3 2 1 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
#! C:\Program Files (x86)\MGLTools-1.5.7\python.exe
#
#
# $Header:
# /mnt/raid/services/cvs/python/packages/share1.5/AutoDockTools/Utilities24/prepare_receptor4.py,v 1.13.6.1 2015/08/26 22:45:31
# sanner Exp $
#
import os

from MolKit import Read
import MolKit.molecule
import MolKit.protein
from AutoDockTools.MoleculePreparation import
AD4ReceptorPreparation

if __name__ == '__main__':
    import sys
    import getopt

    def usage():

```

- Do this step for all the five files

Launch vspipe-gui

If you have followed all steps as described in this tutorial, `vspipe-gui-windows-app.exe` should run successfully. Go to the desktop and click on `vspipe-gui-app.exe` to launch the tool for virtual screening.