

VSpice – GUI Installation Guide for Linux

Accessing and downloading VSpice-GUI repository

- Access the GitHub repository
- Clone or go to the path or Executables/Linux/, and download the repo containing following files
 - *vspice-gui-linux-app* (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-linux-app 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 (<https://www.python.org/downloads/source/>)
2. MGL Tools (<https://ccsb.scripps.edu/mgltools/downloads/>)
3. Autodock tools (*sudo apt-get install autodock-vina*)
4. Rscript (*sudo apt-get install r-base*)
5. Alacarte (*sudo apt-get install alacarte*)
6. Gedit (*sudo apt-get install gedit*)

Step-by-Step guide

Once you have downloaded above mentioned files/directories from the repo, do the following steps:

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

7. You will need to locate the path of MGL tools and find out the path of a file ‘**pythonsh**’
 - a. For example, in current machine, this path is:
`/usr/bin/env /home/rashid/MGLTools-1.5.6/bin/pythonsh`
(This path will be changed depends on where you have installed MGL tools)
8. Give following commands.
 - ◆ `cd vspice-tools/`
 - ◆ `gedit prepare_receptor4.py`
(Change the header as shown in figure above)

- ◆ `gedit prepare_ligand4.py`
(Change the header as shown in figure above)
- ◆ `gedit prepare_dpf4.py`
(Change the header as shown in figure above)
- ◆ `gedit prepare_gpf4.py`
(Change the header as shown in figure above)
- ◆ `gedit summarize_results4.py`
(Change the header as shown in figure above)
- ◆ `sudo cp * /usr/local/bin/`
- ◆ `sudo chmod 777 -R /usr/local/bin/`
- ◆ `unzip vspipe-libraries.zip`
- ◆ `sudo cp -r minimised_libs /usr/local/lib/`
- ◆ `sudo chmod 777 -R /usr/local/lib/minimised_libs/`
- ◆ `alacarte`
- ◆ Make changes shown in figure below
- ◆ Give name
- ◆ Browse to the file `vspipe-gui-linux-app`
- ◆ Check on the option (Launch in Terminal)

Launching Vspipe-GUI

Once you have followed the instructions above, Go to the applications and type on the **vspipe-gui-linux-app** in the search menu, double click the **vspipe-gui-linux-app** icon to launch the VSpice GUI.

