

VSpire – GUI Installation Guide for Mac

Accessing and downloading VSpire-GUI repository

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

Installation of dependencies needed to run VSpire-GUI

1. Python (<https://www.python.org/downloads/macos/>)
2. MGL Tools (<https://ccsb.scripps.edu/mgltools/downloads/>)
3. Rscript (<https://cran.r-project.org/bin/macosx/>)

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 vspire-gui

1. You will need to locate the path of MGL tools and find out the path of a file ‘**pythonsh**’
 - For example, in current machine, this path is:
/Users/lydiatabernero/Downloads/mgltools_1.5.7_MacOS-X/bin/pythonsh
(This path will be changed depends on where you have installed MGL tools)

2. Give following commands.

```
◆ cd vspire-tools/  
◆ open -a TextEdit prepare_receptor4.py  
  (Change the header as shown in figure below)  
◆ open -a TextEdit prepare_ligand4.py  
  (Change the header as shown in figure below)  
◆ open -a TextEdit prepare_dp4.py  
  (Change the header as shown in figure below)
```

- ♦ `open -a TextEdit prepare_gpf4.py`
(Change the header as shown in figure below)
- ♦ `open -a TextEdit summarize_results4.py`
(Change the header as shown in figure below)
- ♦ `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/`

Launching Vspipe-GUI

Once you have followed the instructions above, double click on the **vspipe-gui-mac-app** icon to launch the VSpice GUI.

Old File

```
#!/usr/bin/env /home/rashid/MGLTools-1.5.6/bin/pythonsh
#
#
# $Header: /opt/cvs/python/packages/share1.5/AutoDockTools/Utilities24/prepare_receptor4.py,v 1.5.6.1 2005/09/01 10:10:10 rashid 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():
        "Print helpful, accurate usage statement to stdout."
        print ("Usage: prepare_receptor4.py -r filename")
        print()
        print ("    Description of command...")
        print ("    -r filename")
```

Change the header line with the path as defined in the first step

Update the header line and save it

```
#!/usr/bin/env /Users/lydiatabernero/Downloads/mgltools_1.5.7_MacOS-X/bin/pythonsh
#
#
# $Header: /opt/cvs/python/packages/share1.5/AutoDockTools/Utilities24/prepare_receptor4.py,v 1.5.6.1 2005/09/01 10:10:10 rashid 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():
        "Print helpful, accurate usage statement to stdout."
        print ("Usage: prepare_receptor4.py -r filename")
        print()
        print ("    Description of command...")
```