VSpipe – GUI Installation Guide for Mac

Accessing and downloading VSpipe-GUI repository

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

Installation of dependencies needed to run VSpipe-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 vspipe-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)
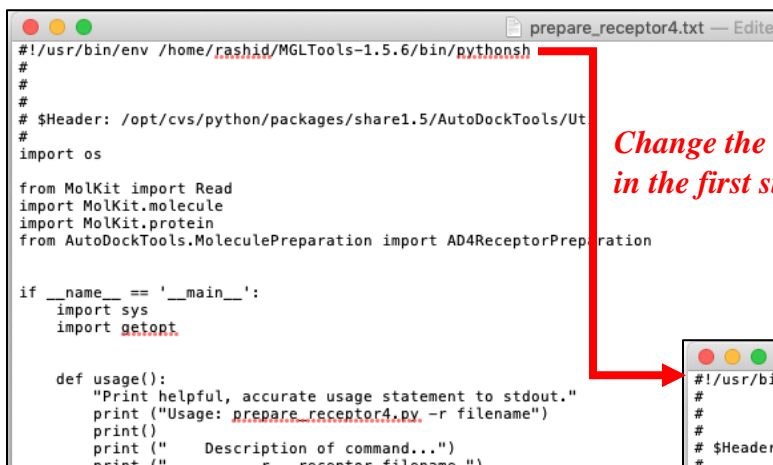

2. Give following commands.

    ```
    ♦ cd vspipe-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_dpf4.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 VSpipe GUI.
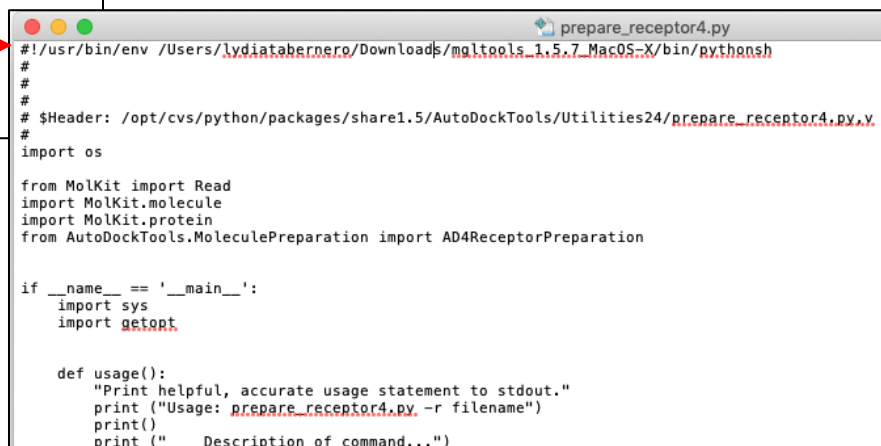
Old File

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

Update the header line and save it