

The "PyDescriptor.py" script has been jointly developed by Dr. Vijay Masand (Amravati, India) and Dr. Vesna Rastija (Osijek, Croatia) under the project INGI-2015-20 funded by Josip Juraj Strossmayer University of Osijek, Croatia. The users can modify and distribute it with the condition to keep the names of original developers and the funding university as it is. It is unlawful to remove the names of original developers and the funding university.

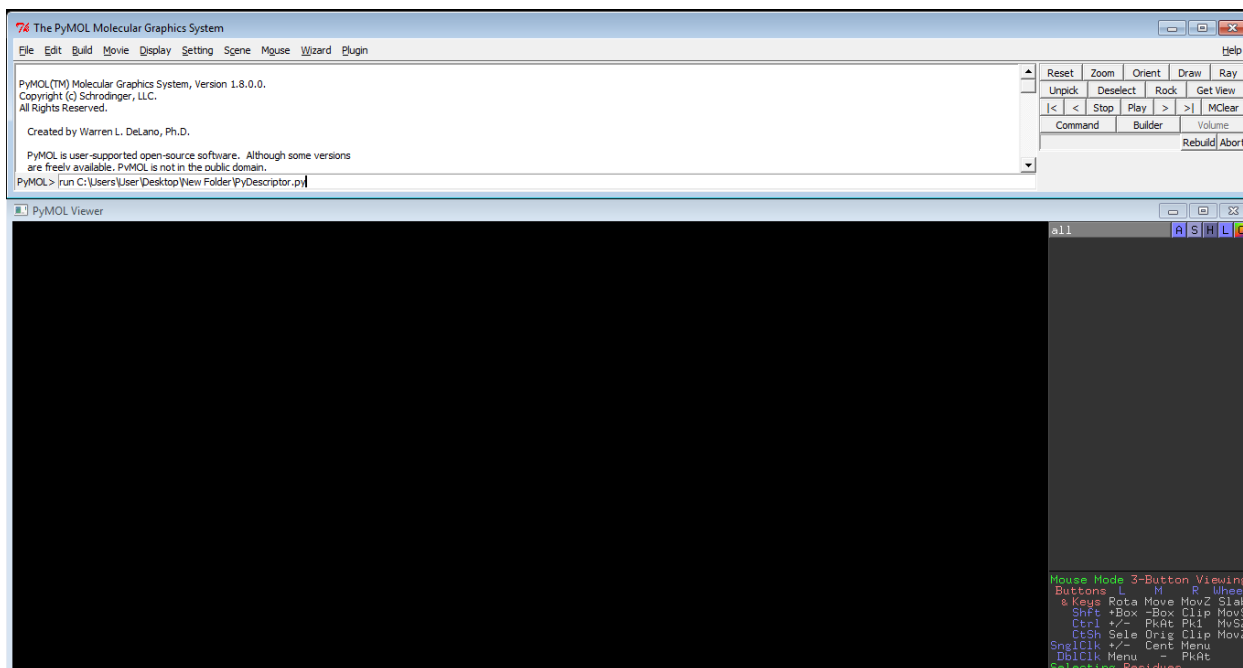
The script has been developed using PyMol 1.8.0.0 and Python 2.7.10 (64 bit) on Windows 7 (64 bit). Though, it has not been tested on other versions of Pymol, Python and other operating systems, but expected to work smoothly without any problem. This script calculates 4653 molecular descriptors for a molecule previously saved in a .mol2 file and saves the output into 'descriptor.csv' file. The 'descriptor.csv' file has been provided with this script and users must keep it in home directory of Python 2.7 (Default C:\Python27). The tutorial is for Windows 7 users.

After downloading this script, keep it in the folder where all the .mol2 files are present. Open PyMol and paste following command in command input area of PyMol:

```
run C:\location of this script\PyDescriptor.py
```

For e.g. suppose all the .mol2 files are in the folder "New Folder" on the "Desktop" of the computer, then the command will look like(Please see the figure also):

```
run C:\Users\User\Desktop\New Folder\PyDescriptor.py
```



After writing above command, press "Enter".

If everything is fine, PyMol will display the progress of completion of calculation of descriptors for a molecule on the screen also. The output visible on the PyMol screen is:

"The data for molecule have been appended to descriptors.csv, file name"