

How to install AutoDock Vina on Ubuntu?

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AutoDock Vina is one of the most popular software in Bioinformatics, known for the molecular docking simulations. I have already explained the docking procedure in my [previous article](#). In this small tutorial, we will learn how to install AutoDock Vina on Ubuntu. Its installation on Ubuntu may be a tedious process, especially for the beginners due to the unfamiliarity of the Linux commands. It is expected to work on any version of Ubuntu, but make sure whether your system supports the 32-bit or 64-bit version. If you face any problem, then feel free to ask. You need a good Internet connection as you will have to download different files. We need to download the following softwares to install AutoDock Vina:

1. MGL Tools (AutoDock Tools are important as they provide the GUI)
2. AutoDock Vina
3. Python

Getting started

It is good to update and upgrade your Ubuntu system first. Log into your Ubuntu system and open the terminal by pressing Ctrl+Alt+T altogether. and type the following commands:

```
$ sudo apt-get update  
$ sudo apt-get upgrade
```

Downloading the files

Now we are going to download the above mentioned files one by one. You can download them either directly by visiting the websites or you can download using the command line as follows. It basically downloads in the 'Downloads' folder, so we will enter into this directory and download the files using command line.

```
$ cd Downloads/  
$ wget http://mgltools.scripps.edu/downloads/tars/releases/REL1.5.6/mgltools_i86Linux2_1.5.6.tar.gz  
$ wget http://vina.scripps.edu/download/autodock_vina_1_1_2_linux_x86.tgz
```

It is good to install python PIL because most of the times it prompts an error for imaging C module during the installation.

```
$ wget http://effbot.org/downloads/Imaging-1.1.7.tar.gz
```

In my case, this issue was not resolved even after installing the imaging C module, then I installed the following library and it resolved my case. If you also get the same error even after installing python imaging library, then try the following:

```
$ sudo apt-get install libjpeg62:i386
```

Installation

Now that we have the tar files in Downloads folder, we will extract and install them one by one. Lets install MGL tools first, and then later the AutoDock Vina. To install them, open the terminal and go to the Downloads folder again.

```
$ cd Downloads  
$ tar xvzf mgltools_i86Linux2_1.5.6.tar.gz
```

This will extract files of mgl tools and create a folder named "mgltools_i86Linux2_1.5.6". Now to install it, we will go into the mgl tools directory.

```
$ cd mgltools_i86Linux2_1.5.6  
$ ./install.sh
```

During installation, a dialog box will prompt on your screen, its the license agreement, so just click "Ok". If everything goes well, then the terminal will show "MGLTools installation complete". It will also ask to create aliases to run them because its a tedious task to write the full path every time we run them. So it is convenient to create aliases which I will tell you a little later, after we finish installation of AutoDock Vina.

We have installed mgl tools on the system, now we will go for AutoDock Vina. To do that, lets go back in our Downloads folder, where we downloaded the tar files.

```
$ cd Downloads/  
$ tar xvzf autodock_vina_1_1_2_linux_x86.tgz
```

After extracting the tar file of AutoDock Vina, you will see a folder in your Downloads directory named "autodock_vina_1_1_2_linux_x86", which consists of a bin folder where you could see two setup files

for vina: “vina” & “vina_split”.

This ends the installation section of our tutorial. Now we have successfully installed AutoDock Vina on Ubuntu. In the following section, I will tell you how to create aliases for the paths.

Creating aliases

If you would see the README file in the bin folder of mgl tools, it shows the paths for running the autodock tools and pymol viewer. Using these paths, we will create aliases.

Open the terminal, go into your home directory, and type the following commands:

```
$ alias adt='sudo /home/Downloads/mgltools_i86Linux2_1.5.6/bin adt'
```

```
$ alias pmv='sudo /home/Downloads/mgltools_i86Linux2_1.5.6/bin pmv'
```

Now, whenever you will type ‘adt’ or ‘pmv’, it will open the autodock vina or pymol viewer respectively.

We are all done! You can perform docking on your Ubuntu system using AutoDock Vina whenever you want. ?

For any query, you can comment below, or email me at muniba@bioinformaticsreview.com.

Reference

Trott, O., & Olson, A. J. (2010). AutoDock Vina: improving the speed and accuracy of docking with a new scoring function, efficient optimization, and multithreading. *Journal of computational chemistry*, 31(2), 455-461.

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