Instructions to Install AutoDock4

Procedure to Install AutoDock4 on Windows OS

1. Download the installer files for **AutoDock suite version 4.2.6**

and **MGL Tools version 1.5.7** from the official **AutoDock** website. Open the URL given here in

any web browser: https://autodock.scripps.edu/

2. Hover the mouse over the **Downloads** link on the left-side of the page. From the options click on

AutoDock4.

3. The page refreshes, from the options on the page, click on the installer file for **AutoDock4**

Windows.

4. **autodocksuite-4.2.6.i86Windows.exe** file gets downloaded to your **Downloads** folder.

5. Go to the **Downloads** folder. Double click on the downloaded **autodocksuite-**

4.2.6.i86Windows.exe file.

6. Click **yes** on the pop-up message asking to give permission to continue the installation.

7. **Choose Install Location** window opens. You will be prompted to choose a custom location or

default location. The default location would be : C:\Program Files (x86)\The Scripps Research

Institute\Autodock\4.2.6.

8. I will choose the default location and click on **Install** button at the bottom-right corner.

9. Close the **set up** window once you get the message that the installation is completed.

10. After the installation is complete go to the C drive Program files and **locate The Scripps**

Research Institute folder.Double-click to open the folder, in side this you will find **Autodock**

folder.

11. Make sure the two executable files **autodock4.exe** and **autogrid4.exe** are present in the folder.

12. Now let us install **AutoDock Tools.** For this we need to download the **MGL** tools which include

ADT. Scroll down the page. There is a message which reads, **To download the graphical user**

interface of AutoDock Tools (ADT) click here , Click on the link.

https://ccsb.scripps.edu/mgltools/

13. You will be directed to another page. Click on **Downloads** link seen on the left-side of the page.

The page refreshes. Click on the installer file corresponding to Windows OS.

mgltools_win32_1.5.7_Setup.exe (80 Mb)

14. The installer file downloads to the **Downloads** folder. Double-click on the downloaded file.

Click **yes** when prompted to continue with the installation.

15. Click **Next** in the MGL Tools Setup window.

16. Accept the terms of license agreement in the **MGL Tools License Agreement** window. Click on

Yes button to continue the installation process.

17. **Choose Destination Location** window opens. Here, you have an option to accept the default

location or browse to choose a new location.

18. Click on **Next** to continue. In the Installing MGL Tools window, click on **Next .**

19. A small pop-up window about commercial usage opens. Read the message and click on **OK**.

20. Installation complete window opens, check the check-boxes for,
Launch PMV
Create Desktop shortcut
Create Quick Launch Shortcut
21. Click on **Finish** button to exit.

22. **AutoDockTools** graphical interface opens. This ensures the successful installation of ADT

Tools. Close the window.

23. Check for desktop short cut for **ADT** Tools.

Procedure to Install AutoDock4 on Ubuntu Linux OS

1. Download the following installer files for **AutoDock suite version 4.2.6**

and **MGL Tools version 1.5.7** from the official **AutoDock** website.

2.   Open the URL given here in any web browser: https://autodock.scripps.edu/

3. Hover the mouse over the **Downloads** link on the left-side of the page. From the options click on

AutoDock4.

4. The page refreshes, click on the installer file for **AutoDock Linux 64 bit**.

5. The compressed tar file, **autodocksuite-4.2.6** downloads to the **Downloads** folder.

6. We need to also download the **MGL** tools which include **ADT**. Scroll down the page. There is a

message which reads, **To download the graphical user interface of AutoDock Tools (ADT) click**

here , Click on the link.

7. You will be directed to another page. https://ccsb.scripps.edu/mgltools/

 Click on **Downloads** link seen on the left-side of the page. The page refreshes. It displays the latest

stable version of MGL tools.

8. Click on **Linux 64 tar ball** installer file. The installer file automatically downloads to your

Downloads folder.

9. For installation of **AutoDock 4.2.6** and **MGL tools 1.5.7**, open the terminal and type the

following commands: (The commands to be typed at the promt on the terminal are given below in

red font color)

Press enter key on keyboard after typing each of the commands shown below.

1. sudo apt-get update

2. sudo apt-get upgrade

3. # Type cd followed by the name of the folder where the autodock4.2.6 installer file is located, if it is Downloads folder type the command as given below.

4. cd Downloads

5. tar xvf autodocksuite-4.2.6-x86_64Linux2.tar

6. cd x86_64Linux2

7. sudo mv autodock4 /usr/local/bin

8. sudo mv autogrid4 /usr/local/bin

9. cd

10. *cd Downloads*

11. *tar xvzf mgltools_x86_64Linux2_1.5.7.tar.gz*

12. *cd mgltools_x86_64Linux2_1.5.7*

13. ./install.sh (During installation, a dialog box with a

message on Commercial usage pops up on the screen. Click Ok to accept)

14. cd ..

15. cd ..

16. gedit ~/.bashrc

17. bashrc file opens in the text editor. Scroll down to the end of the file.

18. Type the following commands. The part of command shown in blue is the path for the **MGL tools 1.5.7** files extracted on your system. Please edit accordingly to include the path for the **MGL tools** on your system.

```
alias adt='sudo /home/username/Downloads/mgltools_x86_64Linux2_1.5.7/bin/adt'
```
```
alias pmv='sudo /home/username/Downloads/mgltools_x86_64Linux2_1.5.7/bin/pmv'
```

19. Save the bashrc file.

20. Type the command given below to source the bashrc file.

source ~/.bashrc

14 .We have completed the step of creating aliases.

15. On the terminal, Type, adt at the prompt and Press Enter. ADT interface opens.

Procedure to Install AutoDock4 on Mac OS

1. Download the following installer files for **AutoDock suite version 4.2.6** and **MGL Tools version 1.5.7** from the official **AutoDock** website.

2. Open the URL given here in any web browser: https://autodock.scripps.edu/

3. Hover the mouse over the **Downloads** link on the left-side of the page. From the options click on **AutoDock4**.

4. The page refreshes, locate the installer file for Mac, **AutoDock4 (Mac OS X)**. Click on it.

5. **Autodocsuite-4.2.6-MacOSX.tar** downloads to your **Downloads** folder.

6. Go to **Finder** and go to **Downloads** folder. Double-click on **Autodocsuite-4.2.6-MacOSX.tar** installer file.

7. The extracted folder **MacOSX** is seen. Double click to open it. Here you will see two files. **Autodoc4** and **autogrid4**.

8. You may need to install **XQuartz** as a prerequisite for **ADT** to work on Mac

9. Download **Xquartz-2.8.5pkg** from given link under quick Download

https://www.xquartz.org/releases/XQuartz-2.8.5.html

9. Go to downloads folder and double-click on the installer file. A pop-up window opens , click on

continue.

10. Click on **continue** button on the install window at the bottom right corner.

11. Click on **agree** in the license agreement window. Click on **continue**.

12. A pop-up asks you to log out of all the applications, click on **continue installation.**

Give your system password when prompted.

13. The installation is successful message appears. Click on **Log Out** button at the bottom right

corner.

14. The system prompts to move the installer to the trash, click on **Move to Trash** button.

This completes the installation of Xquartz.

15. We need to also download the **MGL** tools which include **ADT**. Scroll down the page. There is

a message which reads, **To download the graphical user interface of AutoDock Tools (ADT)**

click here , Click on the link. https://ccsb.scripps.edu/mgltools/

16. You will be directed to another page. Click on **Downloads** link seen on the left-side of the page.

The page refreshes. Scroll down to Version 1.5.7 section and click on the dmg installer file for mac

OS. **(Mgltools-1.5.7-MACOS-X-install.dmg (GUI installer 91 Mb)**

The installer file downloads to your **Downloads** folder.

14. The file automatically opens in a separate window. Double-click on the installation file.

15. A message opens asking for the permission to open. Click on **open** button.

16. Some times an error message, unauthorized app appears, in such case go to **system preferences,**

Go to **security and privacy**. You will see a message at the bottom with **mgl tools** listed .

It was blocked because it shows as unidentified developer. Click on **open anyway**.

In the pop-up window click on **open**. Exit out of security and privacy window.

17. **MGL Tools install Jammer Wizard** opens, click on **Next.**

18. In the MGL Tools license agreement page, **accept** the license agreement and click on **Next.**

19. Successful installation of MGL Tools message appears. Click **Finish** to exit the wizard.

20. Close the **Readme** window.

21. Open the **Finder** and go to **Applications** folder. Locate **MGL Tools-1.5.7** folder.

22. Double-click to open the folder. The folder opens with various tools.

23. Double-Click on **AutoDockTools-1.5.7** to open it.

24. The user interface opens with menus and tools. This completes the installation on Mac OS.

Close the **ADT** interface window.

TROUBLE SHOOTING COMMON ERROR

If an error is displayed while running the autodock or autogrid in the graphical interface, then use

the following strategy :

1. Open command and prompt in window/terminal in linux and run the following commands to

run autodock4 and autogrid4 respectively:

Windows OS

 autogrid4.exe –p file.gpf –l file.glg

autogrid4.exe –p file.dpf –l file.dlg

Linux OS

./autogrid4.exe –p file.gpf –l file.glg

./autogrid4.exe –p file.dpf –l file.dlg