

Installation of AutoDock4 on Linux OS

Spoken Tutorial Project

<https://spoken-tutorial.org>

National Mission on Education through ICT

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Learning Objectives



Learning Objectives

- ▶ **Download AutoDock 4.2.6 installer files**



Learning Objectives

- ▶ **Download AutoDock 4.2.6 installer files**
- ▶ **Install Autodock 4.2.6 on Ubuntu Linux OS**



Learning Objectives

- ▶ **Download AutoDock 4.2.6 installer files**
- ▶ **Install Autodock 4.2.6 on Ubuntu Linux OS**
- ▶ **Install MGL Tools**



Learning Objectives



Learning Objectives

- Create aliases for using AutoDock Tools (ADT) and Python Molecular Viewer (PMV)



Learning Objectives

- ▶ Create aliases for using AutoDock Tools (ADT) and Python Molecular Viewer (PMV)
- ▶ Open the GUI for ADT and PMV



System Requirements



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► **Ubuntu Linux OS v20.04**



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- ▶ **AutoDock v4.2.6**



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- ▶ **Ubuntu Linux OS v20.04**
- ▶ **AutoDock v4.2.6**
- ▶ **MGL Tools v1.5.7**
- ▶ **Google Chrome browser v96.0.4**



System Requirements

- ▶ **Ubuntu Linux OS v20.04**
- ▶ **AutoDock v4.2.6**
- ▶ **MGL Tools v1.5.7**
- ▶ **Google Chrome browser v96.0.4**
- ▶ **Working internet connection**



Pre-requisites



Pre-requisites

► Basic computer skills



Pre-requisites

- ▶ **Basic computer skills**
- ▶ **Linux commands**



Pre-requisites

- ▶ **Basic computer skills**
- ▶ **Linux commands**
- ▶ **For the prerequisite linux tutorials please visit this website**
https://spoken-tutorial.org/tutorial-search/?search_foss=Linux&search_language=English



Files to Download and Website link



Files to Download and Website link

► Autodock suite v4.2.6



Files to Download and Website link

- ▶ **Autodock suite v4.2.6**
- ▶ **MGL Tools v1.5.7**



Files to Download and Website link

- ▶ **Autodock suite v4.2.6**
- ▶ **MGL Tools v1.5.7**
- ▶ **<https://autodock.scripps.edu/>**



Linux Commands for Installation



Linux Commands for Installation

- ▶ The required commands are provided in a text document in the **Additional Reading Material** section



Linux Commands for Installation

- ▶ The required commands are provided in a text document in the **Additional Reading Material** section
- ▶ Please download and save the file



Linux Commands for Installation

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- ▶ Please download and save the file
- ▶ Copy and paste the commands from this document



Summary

In this tutorial we have,

- ▶ **Downloaded AutoDock 4.2.6 installer files from the website**
- ▶ **Installed them using a terminal on Ubuntu Linux 20.04 OS**



Summary

- ▶ Created aliases to use AutoDock Tools (ADT) and Python Molecular Viewer (PMV)
- ▶ Opened the GUI for ADT and PMV



Assignment

As an assignment,

1. Explore the **Projects** tab in the AutoDock website
2. Use the link given below
<https://ccsb.scripps.edu/projects/>
3. Read information about docking given on the page



About the Spoken Tutorial Project

- ▶ Watch the video available at http://spoken-tutorial.org/What_is_a_Spoken_Tutorial
- ▶ It summarises the Spoken Tutorial project



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Spoken Tutorial Workshops

The Spoken Tutorial Project Team

- ▶ Conducts workshops using spoken tutorials
- ▶ Gives certificates to those who pass an online test
- ▶ For more details, please write to contact@spoken-tutorial.org



Answers for THIS Spoken Tutorial

- ▶ Questions in THIS Spoken Tutorial?
- ▶ Visit <https://forums.spoken-tutorial.org>
- ▶ Choose the minute and second where you have the question
- ▶ Explain your question briefly
- ▶ The Spoken Tutorial project will ensure an answer

You will have to register to ask questions



Forum for specific Questions

- ▶ **The Spoken Tutorial forum is for specific questions on this tutorial**
- ▶ **Please do not post unrelated and general questions on them.**
- ▶ **This will help reduce the clutter**
- ▶ **With less clutter, we can use these discussions as instructional material**



Acknowledgements

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