

# Running AutoDock

<https://spoken-tutorial.org>

National Mission on Education through ICT

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# Learning Objectives



# Learning Objectives

- ▶ Open the PDBQT files for receptor and ligand for docking on the ADT interface



# Learning Objectives

- ▶ **Open the PDBQT files for receptor and ligand for docking on the ADT interface**
- ▶ **Perform docking using default docking parameters**



# Learning Objectives

- ▶ Open the PDBQT files for receptor and ligand for docking on the ADT interface
- ▶ Perform docking using default docking parameters
- ▶ Save the output as .dpf file



# Learning Objectives



# Learning Objectives

## ► Run AutoDock



# Learning Objectives

- ▶ **Run AutoDock**
- ▶ **Open the .dlg file to make sure the autodock run is successfully completed**





# System Requirement



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► **Ubuntu Linux OS v20.04**



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- ▶ **AutoDockTools v1.5.7**



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- ▶ **AutoDockTools v1.5.7**
- ▶ **gedit v3.36.2**



# Pre-requisites



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**Learner should be familiar with,**



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**Learner should be familiar with,**

- ▶ **topics in basic bioinformatics**



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**Learner should be familiar with,**

- ▶ **topics in basic bioinformatics**
- ▶ **basic operations on AutoDock Tools interface**





# Code Files

- ▶ The input files required for this tutorial are available in the Code files link



# Code Files

- ▶ **The input files required for this tutorial are available in the Code files link**
- ▶ **Please download and extract the files**



# Code Files

- **Save the input files in your home directory or working directory**



# Code Files

- ▶ **Save the input files in your home directory or working directory**
- ▶ **Make a copy of all the files and then use them for practising**



# Summary

- ▶ Opened the PDBQT files for receptor and ligand for docking on ADT interface
- ▶ Performed docking using default docking parameters
- ▶ Saved the output as .dpf file



# Summary

- ▶ **Ran AutoDock**
- ▶ **Opened the .dlg file to make sure the autodock run is successfully completed**



# Assignment



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**As an assignment,**

- 1. Run autodock for the example 1DWD given in the Examples folder in the Downloads page**
- 2. <https://autodock.scripps.edu/download-autodock4/>**





# About the Spoken Tutorial Project

- ▶ Watch the video available at [http://spoken-tutorial.org/What\\_is\\_a\\_Spoken\\_Tutorial](http://spoken-tutorial.org/What_is_a_Spoken_Tutorial)
- ▶ It summarises the Spoken Tutorial project



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- ▶ It summarises the Spoken Tutorial project
- ▶ If you do not have good bandwidth, you can download and watch it



# 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](mailto: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**



# Acknowledgements

**The Spoken Tutorial project was established by the Ministry of Education, Govt. of India**

