

# Analyzing Docking Runs

<https://spoken-tutorial.org>

National Mission on Education through ICT

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# Learning Objectives



# Learning Objectives

- ▶ Open the dlg file on the ADT panel



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- ▶ **Open the dlg file on the ADT panel**
- ▶ **Open and visualize the most favorable conformations of the ligand**



# Learning Objectives

- ▶ **Open the dlg file on the ADT panel**
- ▶ **Open and visualize the most favorable conformations of the ligand**
- ▶ **Analyze the binding energies of various conformations**



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- ▶ **Analyze clusters of conformations**



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- ▶ **Analyze clusters of conformations**
- ▶ **Open the dlg file using a text editor and analyze the data**





# Learning Objectives

- ▶ **Analyze clusters of conformations**
- ▶ **Open the dlg file using a text editor and analyze the data**
- ▶ **Export the most favorable docking pose as a pdb file**



# 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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- ▶ **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 dlg file on the ADT panel
- ▶ Opened and visualized the most favorable conformations of ligand
- ▶ Analyzed the binding energies of various conformations



# Summary

- ▶ Analyzed clusters of conformations
- ▶ Opened the dlg file using a text editor and analyzed the data
- ▶ Exported the most favorable docking pose as a pdb file



# Assignment





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**As an assignment,**

- 1. Analyze the dlg files generated for 1DWD receptor-ligand complex**
- 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**

