

# Getting Started with Docking

<https://spoken-tutorial.org>

**National Mission on Education through ICT**

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# Learning Objectives



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- ▶ Download ligand and receptor files from the database



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- ▶ **Perform ligand refinement using AutoDockTools (ADT)**



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- ▶ Prepare ligand for docking



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- ▶ Perform ligand refinement using AutoDockTools (ADT)
- ▶ Prepare ligand for docking
- ▶ Save the refined ligand as pdbqt file



# System Requirement



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- ▶ **AutoDockTools v1.5.7**
- ▶ **Google Chrome browser v96.0.4**
- ▶ **Working internet connection**



# Pre-requisites



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**Learner should be familiar with,**

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- ▶ **basic bioinformatics**



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# Adding Hydrogens

This step can be ignored in cases such as:

- ▶ **Quantum mechanical optimization**
- ▶ Draw the 2D structure and convert to 3D in **Open Babel**
- ▶ In the above cases the hydrogens are automatically added



# Summary

- ▶ Downloaded ligand and receptor files from the database
- ▶ Performed the ligand refinement using AutoDockTools (ADT)
- ▶ Prepared the ligand for docking
- ▶ Saved the refined ligand structure as pdbqt file format using ADT



# Assignment-1

**As an assignment,**

- 1. Read about the docking process**
- 2. Use the link given here for more information**

**<https://ccsb.scripps.edu/projects/docking/>**



# Assignment-2

1. Download the ligand and receptor files from the PDB database for 1DWD
2. Do the ligand refinement and create the pdbqt file for 1DWD



# 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**

