Receptor Preparation for Docking

https://spoken-tutorial.org
National Mission on Education through ICT

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Learning Objectives

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▶ **Open the receptor pdb file on the ADT display panel**

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▶ **Delete the water molecules from the receptor structure**

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▶ **Add hydrogens to the receptor structure**

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▶ **Remove the ligand molecule crystallized along with the receptor**

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▶ **Save the current session**

System Requirement

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- **Ubuntu Linux OS v20.04**

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- **AutoDockTools v1.5.7**

Pre-requisites

Learner should be familiar with,

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▶ **topics in basic bioinformatics**

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Learner should be familiar with,

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- ▶ **basic operations on AutoDock Tools interface**

Code Files

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▶ **Make a copy of all the files and then use them for practising**

Summary

- **Opened the receptor pdb file on the ADT display panel**
- **Deleted the water molecules from the receptor structure**
- **Added hydrogens to the receptor structure**

Summary

▶ **Removed the ligand molecule crystallized along with the receptor**

▶ **Saved the current session**

Assignment

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As an assignment,

1. **Practice the same steps with 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**
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► **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**

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**