

Visualizing Docking using UCSF Chimera

<https://spoken-tutorial.org>

National Mission on Education through ICT

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Learning Objectives



Learning Objectives

- ▶ Open the PDB file for the receptor on the Chimera interface



Learning Objectives

- ▶ **Open the PDB file for the receptor on the Chimera interface**
- ▶ **Select and delete solvent and other residues from the receptor structure**



Learning Objectives

- ▶ Add the most preferred docking pose of the ligand to the receptor structure



Learning Objectives

- ▶ Add the most preferred docking pose of the ligand to the receptor structure
- ▶ Show hydrogen bonds and other interactions



Learning Objectives

- ▶ Highlight the active site residues



Learning Objectives

- ▶ **Highlight the active site residues**
- ▶ **Show the receptor-ligand surface and active site pocket**



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**
- ▶ **UCSF Chimera v1.17.2**



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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- ▶ **basic operations on UCSF Chimera interface**



Pre-requisites

Learner should be familiar with,

- ▶ **topics in basic bioinformatics**
- ▶ **basic operations on UCSF Chimera interface**
- ▶ **Please refer to the link below for tutorials on UCSF Chimera series**
<https://spoken-tutorial.org>



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**



Chimera Tools for Visualization



Chimera Tools for Visualization

- ▶ **The two kinds of interactions:**
 - * hydrogen bonds
 - * other polar and nonpolar interactions



Chimera Tools for Visualization

- ▶ **The two kinds of interactions:**
 - * hydrogen bonds
 - * other polar and nonpolar interactions
- ▶ **Visualize the active site pocket and surface properties of the receptor**



Active Site Residues

From the literature, the following residues form much of the ligand binding pocket:

Lys33, Phe80, Glu81, Phe82, Leu83, His84, Gln85, Asp86, Leu134, and Asp145



Conclusion of the Analysis

- ▶ The ligand is interacting mostly with the hydrophobic residues inside the binding pocket



Conclusion of the Analysis

- ▶ The ligand is interacting mostly with the hydrophobic residues inside the binding pocket
- ▶ We found many non bonding interactions with the hydrophobic residues



Conclusion of the Analysis

- ▶ Only a few hydrogen bonds are expected



Conclusion of the Analysis

- ▶ Only a few hydrogen bonds are expected
- ▶ We observed only two hydrogen bonds using the Structure Analysis tool



Summary

- ▶ **Opened the PDB file for the receptor on the Chimera interface**
- ▶ **Selected and deleted solvent and other residues from the receptor structure**



Summary

- ▶ Added the most preferred conformation of ligand obtained after autodock runs to the receptor structure
- ▶ Showed hydrogen bonds and other interactions of the ligand with the receptor



Summary

- ▶ Highlighted the active site residues
- ▶ Showed the receptor-ligand surface and active site pocket



Assignment



Assignment

As an assignment,

- 1. Analyze the dlg files generated for 1DWD receptor-ligand complex using UCSF Chimera**
- 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
- ▶ 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



Acknowledgements

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