

Superimposing Structures

Spoken Tutorial Project

<https://spoken-tutorial.org>

National Mission on Education through ICT

Script: Snehalatha Kaliappan

Video: Madhuri Ganapathi

IIT Bombay

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Learning Objectives



Learning Objectives

In this tutorial, we will learn to,



Learning Objectives

In this tutorial, we will learn to,

- ▶ **Load two or more models on the Jmol panel**



Learning Objectives

In this tutorial, we will learn to,

- ▶ Load two or more models on the Jmol panel
- ▶ Translate and rotate models on the panel



Learning Objectives



Learning Objectives

- ▶ **Superimpose models using script commands**



Learning Objectives

- ▶ **Superimpose models using script commands**
- ▶ **Compare the RMSD score for the superimposition**



System Requirements

Here I am using,



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► Ubuntu Linux OS version 20.04



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- ▶ **Jmol version 14.32.80**



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- ▶ **Ubuntu Linux OS version 20.04**
- ▶ **Jmol version 14.32.80**
- ▶ **Java version 11.0.16**
- ▶ **Working Internet Connection**



Pre-requisites



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Learner should be familiar with,



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- ▶ **Chemistry topics from undergraduate courses**



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Learner should be familiar with,

- ▶ **Chemistry topics from undergraduate courses**
- ▶ **Basic operations of Jmol**



Pre-requisites



Pre-requisites

- For the prerequisite Jmol tutorials please visit this website

https://spoken-tutorial.org/tutorial-search/?search_foss=Jmol+Application&search_language=English



Code Files

- ▶ The input files required for this tutorial are available in the Code files link
- ▶ Please download and extract the files
- ▶ Make a copy of all the files and then use them for practising



Significance of Comparing 3D structures

**Comparing 3D structures of molecules
is useful in,**



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- ▶ **Stereochemical analysis**



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- ▶ **Stereochemical analysis**
- ▶ **Predicting molecular functions**



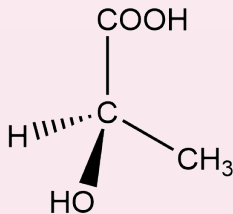
Significance of Comparing 3D structures

Comparing 3D structures of molecules is useful in,

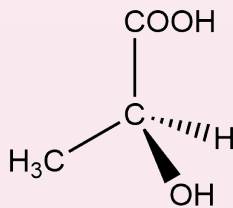
- ▶ **Stereochemical analysis**
- ▶ **Predicting molecular functions**
- ▶ **Drug discovery and design of ligands**



Enantiomers of Lactic Acid



(-)-lactic acid



(+)-lactic acid

Enantiomers



Script Commands

- ▶ Script command with **Compare** command word can be used for superimposition



Script Commands

- ▶ Script command with **Compare** command word can be used for superimposition
- ▶ The command compares two models and reorients the first model relative to the second



Script Commands

- ▶ The reorientation is based on the given atom-atom coordinate pairing



Script Commands

- ▶ The command line with following syntax will be used for the purpose



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- ▶ **compare {model1} {model2}**
SMARTS or SMILES
"smartsString" translate rotate



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- ▶ **compare {model1} {model2}**
SMARTS or SMILES
"smartsString" translate rotate
- ▶ <https://chemapps.stolaf.edu/jmol/docs/#compare>



Script Commands

compare {1.1} {2.1} SMARTS
"O=COH" translate rotate 2.0



RMSD Score

root-mean-square deviation (RMSD):



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- ▶ It is measured in angstrom units



RMSE Score

- ▶ The smaller the RMSE value, the more similar the two structures

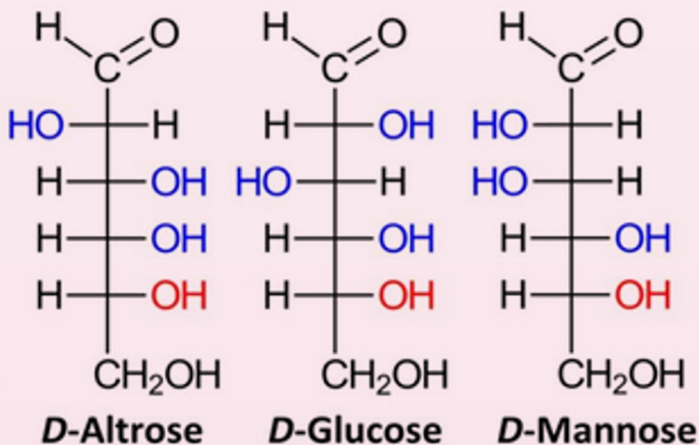


RMDS Score

- ▶ The smaller the RMSD value, the more similar the two structures
- ▶ An RMSD score of $< 2.0 \text{ \AA}$ is observed when the structures have good superimposition



Structures of Carbohydrates



Summary

In this tutorial we learned to,

- ▶ Load two or more models on the Jmol panel
- ▶ Translate and rotate models on the panel



Summary

- ▶ **Superimpose models using script commands**
- ▶ **Compare the RMSD score for the superimposition**



Assignment

- Explore the **compare** command and superimpose models of your choice



About the Spoken Tutorial Project

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- ▶ 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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