

Build Molecules

Spoken Tutorial Project

<http://spoken-tutorial.org>

National Mission on Education through ICT

<http://sakshat.ac.in>

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17 December 2015



Learning Objectives



Learning Objectives

We will learn to:



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We will learn to:

- ▶ **Import molecules from database**



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- ▶ **Import molecules from database**
- ▶ **Rotate, zoom in and zoom out**



Learning Objectives

We will learn to:

- ▶ **Import molecules from database**
- ▶ **Rotate, zoom in and zoom out**
- ▶ **Build molecules on the Panel**
- ▶ **Set up force field and optimize geometry**



Learning Objectives



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- ▶ Measure bond lengths, bond angles, dihedral angles
- ▶ Show fragment library



System Requirement



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- ▶ **Ubuntu Linux OS v 14.04**



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- ▶ **Avogadro v 1.1.1**



Pre-requisites



Download Link



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- ▶ To download Avogadro use the link sourceforge.net/projects/avogadro



Summary

- ▶ Import molecules from database
- ▶ Rotate, zoom in and zoom out
- ▶ Build molecules on the Panel
- ▶ Set up force field and optimize geometry



Summary

- ▶ Measure bond lengths, bond angles, dihedral angles
- ▶ Show fragment library
- ▶ Build DNA molecules and Peptides



Assignment

1. Create a protein sequence using the following amino acid residues:
Glu, Leu, Asn, Cys, His
2. Optimize the geometry using UFF force field
3. Save the image as .cml file



Assignment

1. Build RNA sequence using the Nucleic acids: AUGC
2. Optimize geometry using MMFF94 force field
3. Save the image as .cml file




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
- ▶ If you do not have good bandwidth, you can download and watch it



Acknowledgements

- ▶ Spoken Tutorial Project is a part of the Talk to a Teacher project
 - ▶ It is supported by the National Mission on Education through ICT, MHRD, Government of India
 - ▶ More information on this Mission is available at <http://spoken-tutorial.org/NMEICT-Intro>
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- The logo of Spoken Tutorial, featuring a stylized orange and black circular design with white curved lines.

