

# Build Molecules

**Spoken Tutorial Project**

<http://spoken-tutorial.org>

**National Mission on Education through ICT**

<http://sakshat.ac.in>

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# Learning Objectives



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# Learning Objectives

**We will learn to:**



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# Learning Objectives

**We will learn to:**

- ▶ **Import molecules from database**



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**We will learn to:**

- ▶ **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**



# 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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# Learning Objectives

- ▶ Measure bond lengths, bond angles, dihedral angles



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# Learning Objectives

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



# Learning Objectives

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



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# System Requirement



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# System Requirement

- ▶ **Ubuntu Linux OS v 14.04**





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- ▶ **Ubuntu Linux OS v 14.04**
- ▶ **Avogadro v 1.1.1**
- ▶ **Working Internet connection**



# Pre-requisites



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# Download Link



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- ▶ To download Avogadro use the link [sourceforge.net/projects/avogadro](https://sourceforge.net/projects/avogadro)





# Summary

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



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# 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



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# 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](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



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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](mailto:contact@spoken-tutorial.org)



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# 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>

