

# Surface Properties

Talk to a Teacher

<http://spoken-tutorial.org>

National Mission on Education through ICT

<http://sakshat.ac.in>

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# Learning Objectives



# Learning Objectives

- ▶ **Show surfaces for protein and DNA structures**



# Learning Objectives

- ▶ Show surfaces for protein and DNA structures
- ▶ Create images of protein surface colored by:



# Learning Objectives

- ▶ Show surfaces for protein and DNA structures
- ▶ Create images of protein surface colored by:
  - ▶ **Amino acid hydrophobicity**



# Learning Objectives

- ▶ Show surfaces for protein and DNA structures
- ▶ Create images of protein surface colored by:
  - ▶ Amino acid hydrophobicity
  - ▶ Electrostatic Potential



# Pre-requisites



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- ▶ **Chimera interface**



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- ▶ **Chimera interface**
- ▶ <http://spoken-tutorial.org>



# System Requirement



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- ▶ **Ubuntu OS version 14.04**



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- ▶ **Mozilla firefox browser 42.0**



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- ▶ **Working internet connection**



# Protein Surface



# Protein Surface

**Proteins generally interact with other proteins and molecules through their surface regions**



# Protein Surface



# Protein Surface

Representing a protein by its molecular surface helps in:

- ▶ **Study of protein folding**



# Protein Surface

Representing a protein by its molecular surface helps in:

- ▶ Study of protein folding
- ▶ Prediction of biomolecular recognition



# Protein Surface

Representing a protein by its molecular surface helps in:

- ▶ Study of protein folding
- ▶ Prediction of biomolecular recognition
- ▶ **Detection of drug binding cavities**



# Protein Surface

Representing a protein by its molecular surface helps in:

- ▶ Study of protein folding
- ▶ Prediction of biomolecular recognition
- ▶ Detection of drug binding cavities
- ▶ **Molecular Graphics**



# Summary



# Summary

- ▶ **Show Amino acid hydrophobicity surface and Electrostatic Potential surface for protein and DNA structures**
- ▶ **Create high quality images for publication using different viewing settings**



# Assignment



# Assignment

- ▶ Show **amino acid hydrophobicity surface** and **electrostatic potential surface** for the structure of **Human hemoglobin (PDB code: 2dn1)**
- ▶ Color the hem ligand **green**



# 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



# 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)



# 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>

