

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



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- ▶ **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



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- ▶ **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
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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



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- ▶ 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>

