

# PDB File Format and Website

**Spoken Tutorial Project**

**<https://spoken-tutorial.org>**

**National Mission on Education through ICT**

**<http://sakshat.ac.in>**

**Rani Parvathy  
IIT Bombay**

**9 August 2021**



# Learning Objectives



# Learning Objectives

- ▶ **About PDB file format for molecular structure**



# Learning Objectives

- ▶ **About PDB file format for molecular structure**
- ▶ **Protein Data Bank (PDB) website**



# Learning Objectives

- ▶ **About PDB file format for molecular structure**
- ▶ **Protein Data Bank (PDB) website**
- ▶ **Download a pdb file from PDB website**



# Learning Objectives

- ▶ **About PDB file format for molecular structure**
- ▶ **Protein Data Bank (PDB) website**
- ▶ **Download a pdb file from PDB website**
- ▶ **About FASTA file format**



# System Requirements



# System Requirements

► **Ubuntu Linux v20.04 OS**





# System Requirements

- ▶ **Ubuntu Linux v20.04 OS**
- ▶ **Firefox web browser v92**



# System Requirements

- ▶ **Ubuntu Linux v20.04 OS**
- ▶ **Firefox web browser v92**
- ▶ **Gedit v3.36.2**



# System Requirements

- ▶ **Ubuntu Linux v20.04 OS**
- ▶ **Firefox web browser v92**
- ▶ **Gedit v3.36.2**
- ▶ **A working internet connection to access the PDB website**



# Pre-requisites



# Pre-requisites

**To follow this tutorial**



# Pre-requisites

## To follow this tutorial

- ▶ **Learner must be familiar with basic computer skills**



# Pre-requisites

## To follow this tutorial

- ▶ **Learner must be familiar with basic computer skills**
- ▶ **For pre-requisite tutorials, please visit this site**

**<https://spoken-tutorial.org/>**



# Downloaded Gromacs Tarball





# Downloaded Gromacs Tarball

**Files used in this tutorial, can be found in the**



# Downloaded Gromacs Tarball

**Files used in this tutorial, can be found in the**

- ▶ **Downloaded and extracted tarball directory used for Gromacs installation**



# Protein Data Bank

- ▶ Protein Data Bank is a repository of 3D structural data of biomolecules



# Protein Data Bank

- ▶ Protein Data Bank is a repository of 3D structural data of biomolecules
- ▶ <https://www.rcsb.org/>



# Protein Data Bank

- ▶ Protein Data Bank is a repository of 3D structural data of biomolecules
- ▶ <https://www.rcsb.org/>
- ▶ The structures are determined by X-ray diffraction, NMR & electron microscopy



# Protein Data Bank

- ▶ Protein Data Bank is a repository of 3D structural data of biomolecules
- ▶ <https://www.rcsb.org/>
- ▶ The structures are determined by X-ray diffraction, NMR & electron microscopy



# Protein Data Bank

- ▶ Protein Data Bank is a repository of 3D structural data of biomolecules
- ▶ <https://www.rcsb.org/>
- ▶ The structures are determined by X-ray diffraction, NMR & electron microscopy



# Protein Data Bank





## Atomic resolution structures for



## Atomic resolution structures for

### ► Proteins, DNA & RNA



## Atomic resolution structures for

- ▶ Proteins, DNA & RNA
- ▶ Carbohydrates & lipids



## Atomic resolution structures for

- ▶ Proteins, DNA & RNA
- ▶ Carbohydrates & lipids
- ▶ **Several ligand molecules**



## Atomic resolution structures for

- ▶ Proteins, DNA & RNA
- ▶ Carbohydrates & lipids
- ▶ Several ligand molecules



## Atomic resolution structures for

- ▶ Proteins, DNA & RNA
- ▶ Carbohydrates & lipids
- ▶ Several ligand molecules

are available here



# Summary

- ▶ **The PDB file format**
- ▶ **The PDB website**
- ▶ **FASTA file format**
- ▶ **Header details in the PDB file**
- ▶ **Downloaded a pdb file**



# Assignment





# Assignment

- ▶ **Go through the PDB website**
- ▶ **Familiarize with more details given for the PDB deposition**
- ▶ **Go through the header details of the file that is downloaded**



# Assignment



# Assignment

**Go through the given IDs from PDB website for enzyme DHFR and its complexes**

- ▶ **2L28 for apo enzyme and multiple conformers**
- ▶ **1DIS for binary complex**
- ▶ **3DAT for ternary complex**



# Assignment



# Assignment

- ▶ Notice the presence and absence of hydrogen atoms in the structure files
- ▶ Familiarize with
  - ▶ Conformational changes in the enzyme
  - ▶ Hydrogen bonding with ligands



# About the Spoken Tutorial Project

- ▶ Watch the video available at [https://spoken-tutorial.org/What\\_is\\_a\\_Spoken\\_Tutorial](https://spoken-tutorial.org/What_is_a_Spoken_Tutorial)
- ▶ It summarises the Spoken Tutorial project



# About the Spoken Tutorial Project

- ▶ Watch the video available at [https://spoken-tutorial.org/What\\_is\\_a\\_Spoken\\_Tutorial](https://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



# 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)**





# Forum questions

- ▶ 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

**Spoken Tutorial Project is supported by**

- ▶ **National Mission on Education through ICT (NMEICT)**
- ▶ **Pandit Madan Mohan Malaviya National Mission on Teachers and Teaching (PMMMNMTT)**

**MoE, Government of India**

