Sr. No	Lecture Title	Description	Category	Durations
	Segment 6: Molecular Dynamics & Simulation			
1	Getting Started With Molecular Dyanmics Simulation - Pre-processing of Protein Structure and Removal of Unncessary Structural Features	• Introduction to GROMACS and its installation. • Pre-processing of the protein structure and removal of unnecessary structural features.	Protein Simulation	12:33
2	pdb2gmx - Construction of Topology File for Simulation	• Introduction to pdb2gmx tool of GROMACS. • Construction of topology file for simulation.	Protein Simulation	9:00
3	Defining a Solvant Box for Simulation	• Introduction to GROMACS for defining solvant box. • Definig a solvant box to prepare the protein for simulation.	Protein Simulation	4:14
4	Solvation - Adding Water Molecules in Solvant Box	• Introduction to GROMACS for defining solvant box. • Adding water molecules in solvant box to prepare the protein for simulation.	Protein Simulation	5:30
5	Generating Input Run File Replacement of Water Molecues With Ions	• Generating input run file. • Replacing the water molecules with ions for protein simulation.	Protein Simulation	6:55
6	genion - Replacement of Water Molecules With Ions	• Introduction to genioin tool of GROMACS. • Replacing the water molecules with ions for protein simulation.	Protein Simulation	4:18
7	Energy Minimization - Relaxing and Fixing the Structure for Simulation	• Introduction to gmx energy tool of GROMACS. • Relaxing and fixing the structure for protein simulation.	Protein Simulation	11:25
8	GRACE - Visualization and Analysis of Minimized Structure	• Introduction to gmgrace tool of GROMACS. • Visualization and analysis of minimized structure of the protein.	Protein Simulation	4:11

9	Equibiliration of Protein Structure NVT ENSEMBLE Phase 1	• Introduction to nvt tool of GROMACS. • Phase 1 of NVT ENSEMBLE to equilibrate the protein structure.	Protein Simulation	8:37
10	Equibiliration of Protein Structure NPT ENSEMBLE Phase 2	• Introduction to nvt tool of GROMACS. • Phase 2 of NVT ENSEMBLE to equilibrate the protein structure.	Protein Simulation	8:09
11	mdrun - Executing Simulation Analysis	• Introduction to mdrun tool of GROMACS. • Execution of MD simulation on the protein structure.	Protein Simulation	3:46