

Days	Name	Durations	Category	Main Category
1	Getting Started With Molecular Dynamics Simulation - Pre-processing of Protein Structure and Removal of Unnecessary Structural Features	12:33	Protein Structure Preparation	Molecular Dynamics Simulations: GROMACS
2	pdb2gmx - Construction of Topology File for Simulation	9:00	Protein Structure Preparation	Molecular Dynamics Simulations: GROMACS
3	Defining a Solvant Box for Simulation	4:14	Protein Structure Preparation	Molecular Dynamics Simulations: GROMACS
4	Solvation - Adding Water Molecules in Solvant Box	5:30	Protein Structure Preparation	Molecular Dynamics Simulations: GROMACS
5	Generating Input Run File Replacement of Water Molecules With Ions	6:55	Protein Structure Preparation	Molecular Dynamics Simulations: GROMACS
6	genion - Replacement of Water Molecules With Ions	4:18	Protein Structure Preparation	Molecular Dynamics Simulations: GROMACS
7	Energy Minimization - Relaxing and Fixing the Structure for Simulation	11:25	Energy Minimization	Molecular Dynamics Simulations: GROMACS
8	GRACE - Visualization and Analysis of Minimized Structure	4:11	Minimized Structure Visualization	Molecular Dynamics Simulations: GROMACS
9	Equilibration of Protein Structure NVT ENSEMBLE Phase 1	8:37	NVT Ensemble	Molecular Dynamics Simulations: GROMACS
10	Equilibration of Protein Structure NPT ENSEMBLE Phase 2	8:09	NPT Ensemble	Molecular Dynamics Simulations: GROMACS
11	mdrun - Executing Simulation Analysis	3:46	Simulation Execution	Molecular Dynamics Simulations: GROMACS