WORKSHEET

Topic	Task	Commands
Appendix-1	Unzip	tar -zxvf filename.zip
	Directory	mkdir dir1 cd dir1
	Sub-directory	mkdir dir2
	Copy	cp molecule dir2
Appendix-2	Download	wget link
	Visualize	VMD *.pdb
Appendix-3	GROMACS file creation	1. gmx pdb2gmx -f *.pdb -o *.gro 2. VMD *.gro 3. vi topol.top
	Simulation box	1. gmx editconf -f *.gro -o box.gro -c -d 1.0 -bt cubic 2. VMD box.gro 3. vi topol.top
	Solvation	1. gmx solvate -cp box.gro -cs spc216.gro -o solv.gro -p topol.top 2. VMD solv.gro 3. vi topol.top (observe HOH)
	Neutralization	1. cp *.mdp iGEM folder 2. vi ions.mdp 3. gmx grompp -f ions.mdp -c solv.gro -p topol.top -o ions.tpr 4. gmx genion -s ions.tpr -o solv_ions.gro -p topol.top -pname NA -nname CL -neutral 5. VMD solv_ions.gro 6. vi topol.top (observe NA and CL ions)
	Energy minimization	1. vi minim.mdp 2. gmx grompp -f minim.mdp -c solv_ions.gro -p topol.top -o minim.tpr 3. ssh rosalind-n* (2-7) 4. gmx mdrun -v -deffnm minim 5. gmx energy -f minim.edr -o potential.xvg 6. scp potential.xvg system-*@IP: 7. xmgrace potential.xvg
	NVT Equilibration	1. gmx grompp -f nvt.mdp -c minim.gro -r minim.gro -p

		topol.top -o nvt.tpr 2. gmx mdrun -v -deffnm nvt
	NPT Equilibration	1. gmx grompp -f npt.mdp -c minim.gro -r minim.gro -p topol.top -o npt.tpr 2. gmx mdrun -v -deffnm npt