Commands to Analyze the Molecular Dynamics Simulation Data

Step-1: Bringing Protein to the center of the box

```
gmx trjconv -s md.tpr -f md.xtc -o md_center.xtc -pbc mol -center
```

Step-2: Calculation of RMSD

```
gmx rms -s md.tpr -f md_center.xtc -o rmsd.xvg -tu ns
```

Step-3: Calculation of RMSF

```
gmx rmsf -s md.tpr -f md_center.xtc -o rmsf.xvg -res
```

Step-4: Calculation of Radius of Gyration

```
gmx gyrate -s md.tpr -f md_center.xtc -o gyrate.xvg
```

Step-5: Calculation of Total Number of Hydrogen bonds

```
gmx hbond -s md.tpr -f md_center.xtc -num hydrogen.xvg -tu ns
```

Step-6: Calculation of Total Solvent Accessible Surface Area

```
gmx sasa -s md.tpr -f md_center.xtc -o area.xvg -tu ns
```