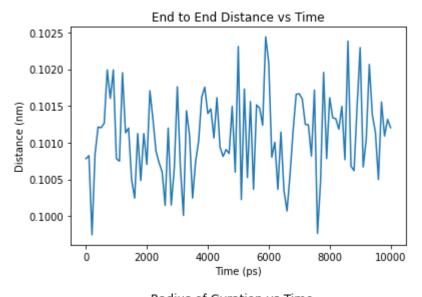
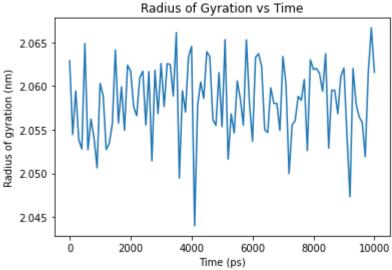
10/12/22, 4:40 PM Pt_1_plots

```
#import Modules
In [24]:
          import numpy as np
          import matplotlib.pyplot as plt
          import mdtraj as md
          #Load xtc Files
          traj = md.load_xtc('trp_cage_fit.xtc', top='step5_9.gro')
          # Plot End to End Distance against Time, with title
          plt.plot(traj.time, md.compute_distances(traj, [[0, 1]]))
          plt.xlabel('Time (ps)')
          plt.ylabel('Distance (nm)')
          plt.title('End to End Distance vs Time')
          plt.show()
          # Plot Radius of Gyration against Time
          plt.plot(traj.time, md.compute_rg(traj))
          plt.xlabel('Time (ps)')
          plt.ylabel('Radius of gyration (nm)')
          plt.title('Radius of Gyration vs Time')
          plt.show()
```





```
In [ ]:
```