

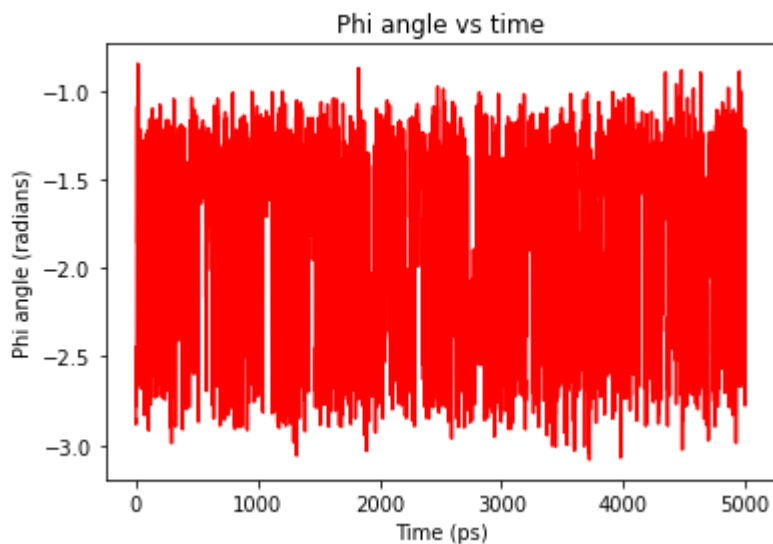
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In [2]: import mdtraj as md
import numpy as np

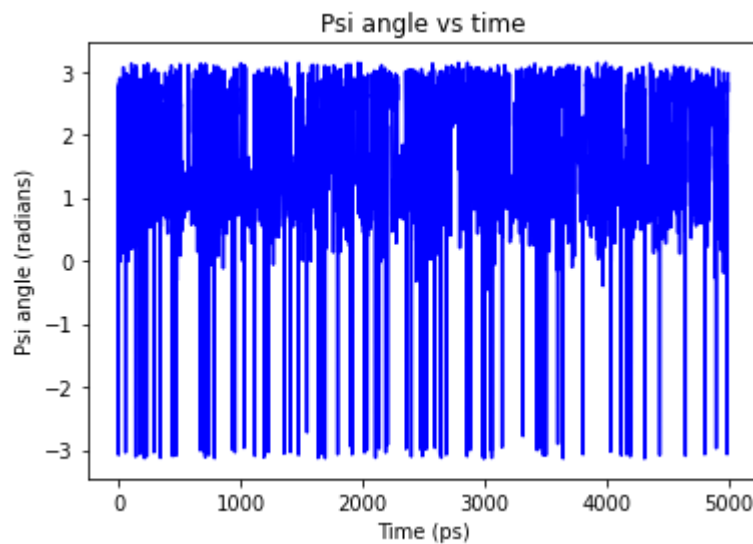
# Load the trajectory
traj = md.load('md_adp_5.trr', top='md_adp_5.gro')

#compute phi and psi dihedral angles for each frame
phi = md.compute_phi(traj)
psi = md.compute_psi(traj)

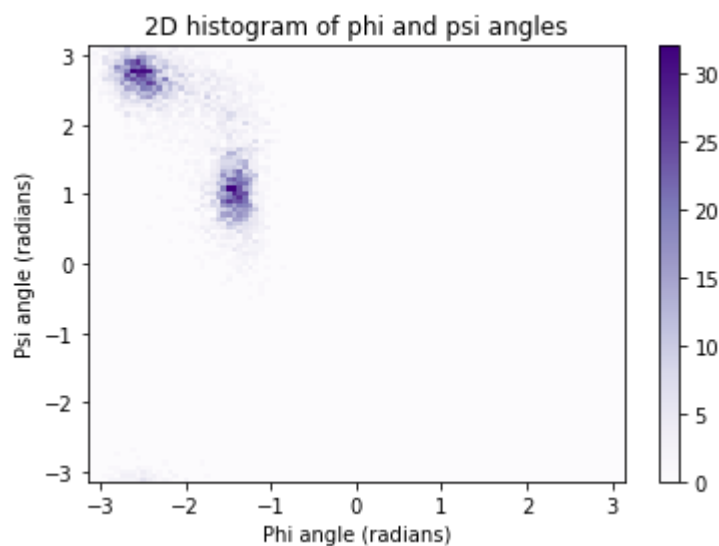
#plot phi angle vs time with title and axis labels
import matplotlib.pyplot as plt
plt.plot(phi[1], 'r')
plt.title('Phi angle vs time')
plt.xlabel('Time (ps)')
plt.ylabel('Phi angle (radians)')
plt.show()

#plot psi angle vs time with title and axis labels
plt.plot(psi[1], 'b')
plt.title('Psi angle vs time')
plt.xlabel('Time (ps)')
plt.ylabel('Psi angle (radians)')
plt.show()
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In [10]: #plot histogram of phi and psi angles
plt.hist2d(phi[1][:,0], psi[1][:,0], bins=100, cmap='Purples', range = [[-np.pi, np.pi]
plt.title('2D histogram of phi and psi angles')
plt.xlabel('Phi angle (radians)')
plt.ylabel('Psi angle (radians)')
plt.colorbar()
plt.show()
```



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In [ ]:
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