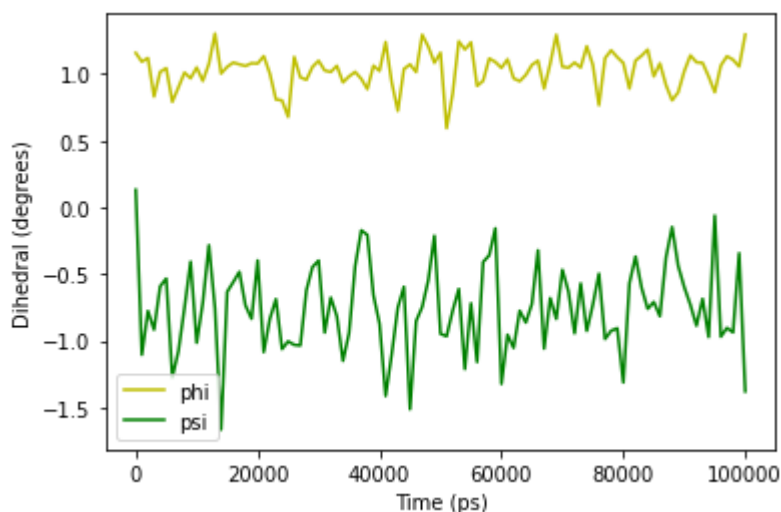


```
In [1]: #import modules

import numpy as np
import matplotlib.pyplot as plt
import mdtraj as md

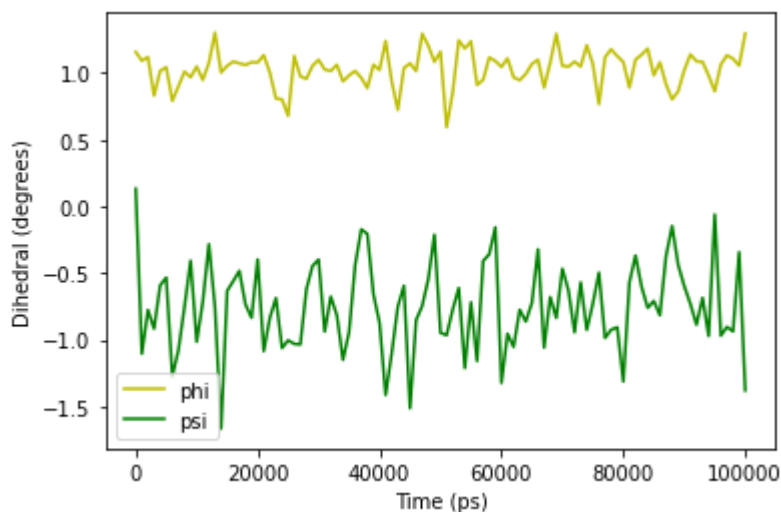
#Read in the data from the COLVAR_B file
data = np.loadtxt('COLVAR_B')

#plot phi and psi dihedrals for every 1000 steps over time with colors and labels
plt.plot(data[:,1000,0], data[:,1000,1], 'y', label='phi')
plt.plot(data[:,1000,0], data[:,1000,2], 'g', label='psi')
plt.xlabel('Time (ps)')
plt.ylabel('Dihedral (degrees)')
plt.legend()
plt.show()
```



```
In [2]: #Use mdtraj to compute the phi and psi dihedrals from traj_comp.xtc
traj = md.load('traj_comp.xtc', top='confout.gro')
phi, psi = md.compute_phi(traj), md.compute_psi(traj)

#plot dihedrals over COLVAR_B over time
plt.plot(data[:,1000,0], phi[1][:,1000,0], 'y', label='phi')
plt.plot(data[:,1000,0], psi[1][:,1000,0], 'g', label='psi')
plt.xlabel('Time (ps)')
plt.ylabel('Dihedral (degrees)')
plt.legend()
plt.show()
```



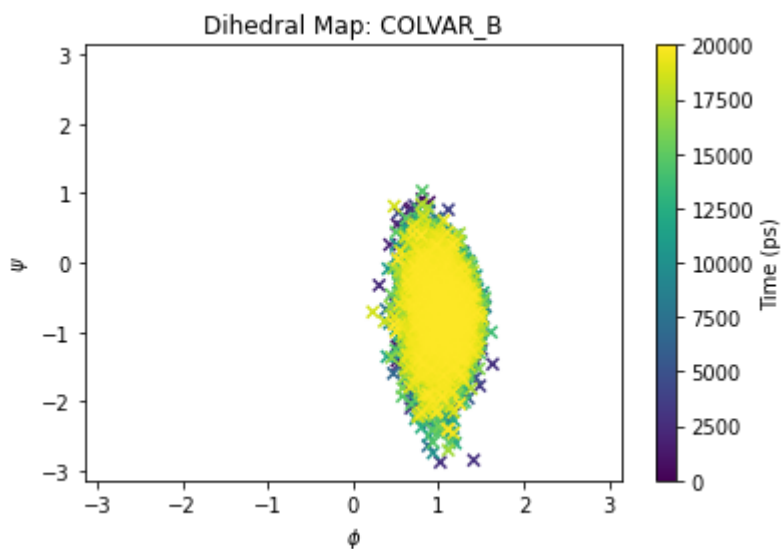
```
In [11]: print("Std_Dev_phi_COLVAR_B =", np.std(phi[1]))
         print("Std_Dev_psi_COLVAR_B =", np.std(psi[1]))
```

```
Std_Dev_phi_COLVAR_B = 0.13238177
Std_Dev_psi_COLVAR_B = 0.34453443
```

```
In [13]: # ramachandran plot using traj_A
         psi_indices, phi_indices = [4, 6, 8, 14], [6, 8, 14, 16]
         angles = md.compute_dihedrals(traj, [phi_indices, psi_indices])

         from pylab import *
         from math import pi

         figure()
         title('Dihedral Map: COLVAR_B')
         scatter(angles[:, 1], angles[:, 0], marker='x', c=traj.time)
         cbar = colorbar()
         cbar.set_label('Time (ps)')
         xlabel(r'$\phi$')
         ylabel(r'$\psi$')
         xlim(-pi, pi)
         ylim(-pi, pi)
         show()
```



```
In [ ]:
```

