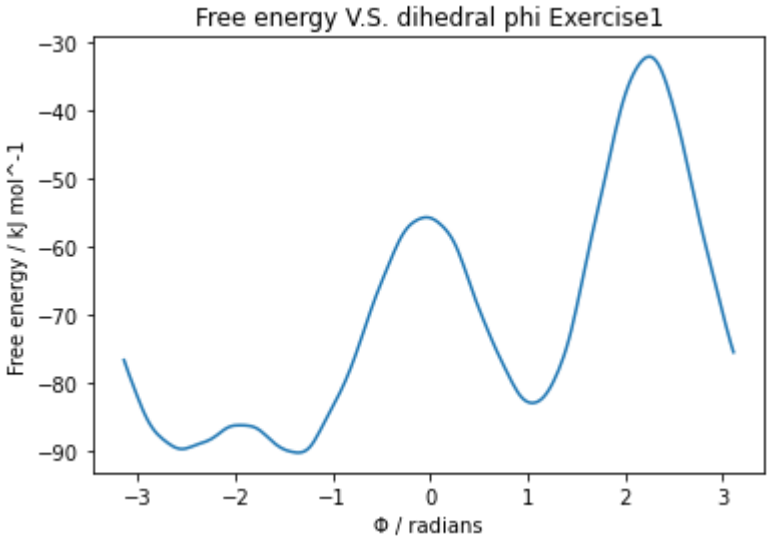
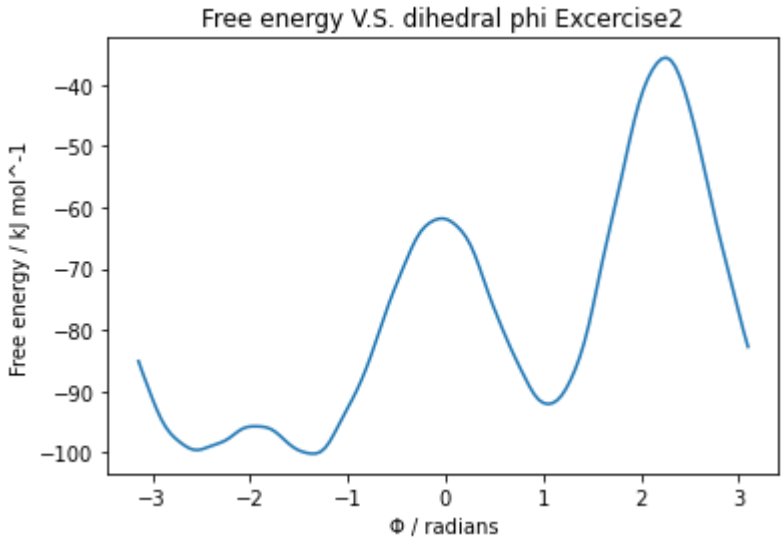
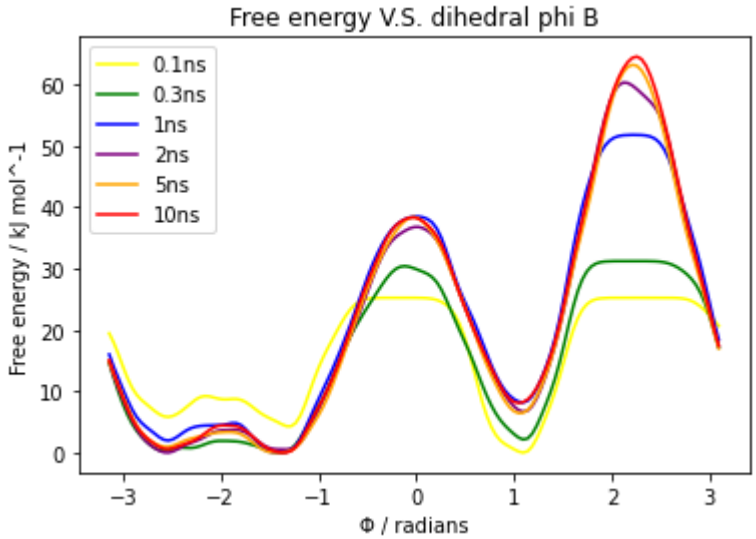
In [3]:
```
#Exercise 1
import pandas as pd
from matplotlib import pyplot as plt
import mdtraj as md
import numpy as np

phi, energy, unknown = np.loadtxt('COLVAR_B.grid.dat', unpack=True)
plt.plot(phi, -energy)


plt.xlabel('Φ / radians')
plt.ylabel('Free energy / kJ mol^-1')
plt.title('Free energy V.S. dihedral phi Exercise1')
plt.show()

#Exercise 2
phi, energy, unknown = np.loadtxt('fes.dat', unpack=True)

plt.plot(phi, energy)

plt.xlabel('Φ / radians')
plt.ylabel('Free energy / kJ mol^-1')
plt.title('Free energy V.S. dihedral phi Excercise2')
plt.show()
```



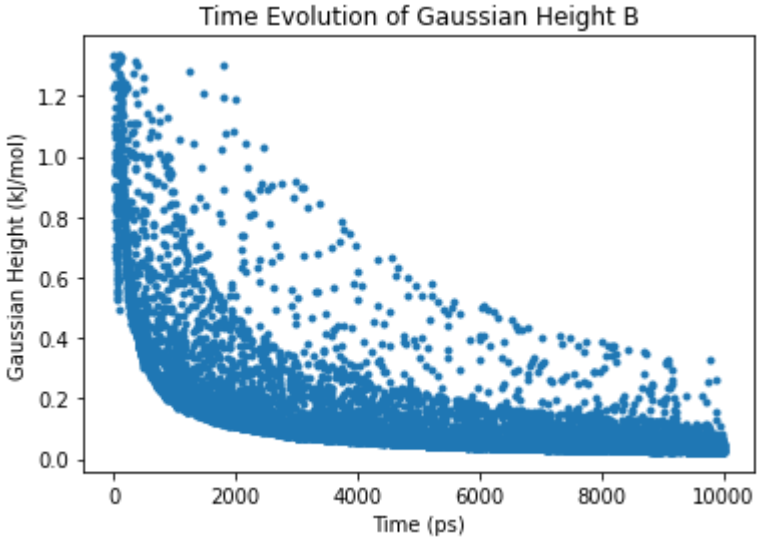


In [11]:
```
# load files fes_1.dat, fes_3.dat, fes_10.dat, fes_20.dat, fes_50.dat, fes_100.dat
fes_1a = np.genfromtxt('/home/kjt9860/compclass/comp-lab-class/comp-lab-class/Week6/Inp
fes_3a = np.genfromtxt('/home/kjt9860/compclass/comp-lab-class/comp-lab-class/Week6/Inp
fes_10a = np.genfromtxt('/home/kjt9860/compclass/comp-lab-class/comp-lab-class/Week6/In
fes_20a = np.genfromtxt('/home/kjt9860/compclass/comp-lab-class/comp-lab-class/Week6/In
fes_50a = np.genfromtxt('/home/kjt9860/compclass/comp-lab-class/comp-lab-class/Week6/In
fes_100a = np.genfromtxt('/home/kjt9860/compclass/comp-lab-class/comp-lab-class/Week6/I

# plot free energy as a function of phi using columns 0 and 1
plt.plot(fes_1a[:,0], fes_1a[:,1], label='0.1ns', color='yellow')
plt.plot(fes_3a[:,0], fes_3a[:,1], label='0.3ns', color='green')
plt.plot(fes_10a[:,0], fes_10a[:,1], label='1ns', color='blue')
plt.plot(fes_20a[:,0], fes_20a[:,1], label='2ns', color='purple')
plt.plot(fes_50a[:,0], fes_50a[:,1], label='5ns', color='orange')
plt.plot(fes_100a[:,0], fes_100a[:,1], label='10ns', color='red')
plt.xlabel('Φ / radians')
plt.ylabel('Free energy / kJ mol^-1')
plt.title('Free energy V.S. dihedral phi B')
plt.legend()
plt.show()
```

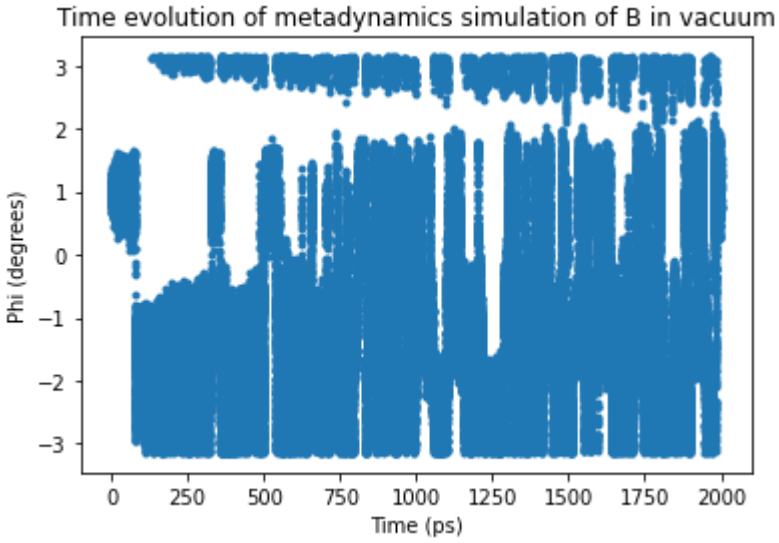


In [12]:
```
data = np.genfromtxt('/home/kjt9860/compclass/comp-lab-class/comp-lab-class/Week6/Input
```

```
plt.plot(data[:,0], data[:,3], '.')
plt.xlabel('Time (ps)')
plt.ylabel('Gaussian Height (kJ/mol)')
plt.title('Time Evolution of Gaussian Height B')
plt.show()
```



In [13]:
```
data_1 = np.genfromtxt('/home/kjt9860/compclass/comp-lab-class/comp-lab-class/Week6/Inp

plt.plot(data_1[:100000,0], data_2[:100000,1], '.')
plt.xlabel('Time (ps)')
plt.ylabel('Phi (degrees)')
plt.title('Time evolution of metadynamics simulation of B in vacuum')
plt.show()
```



In [ ]: