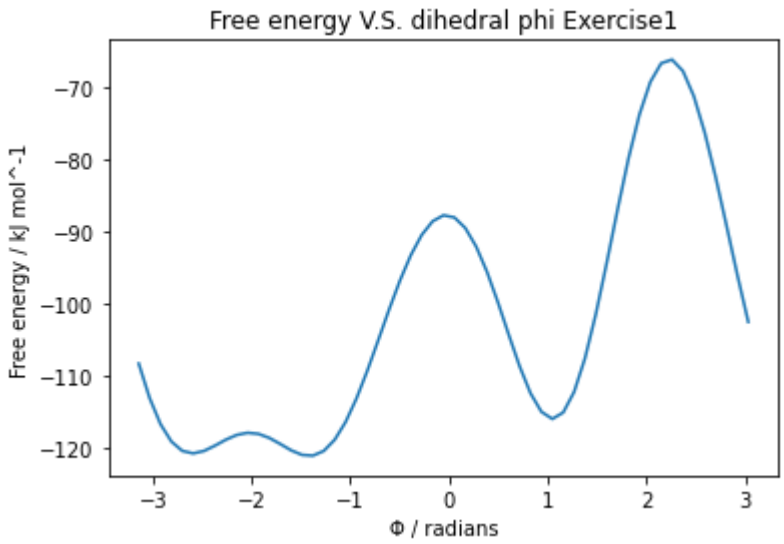
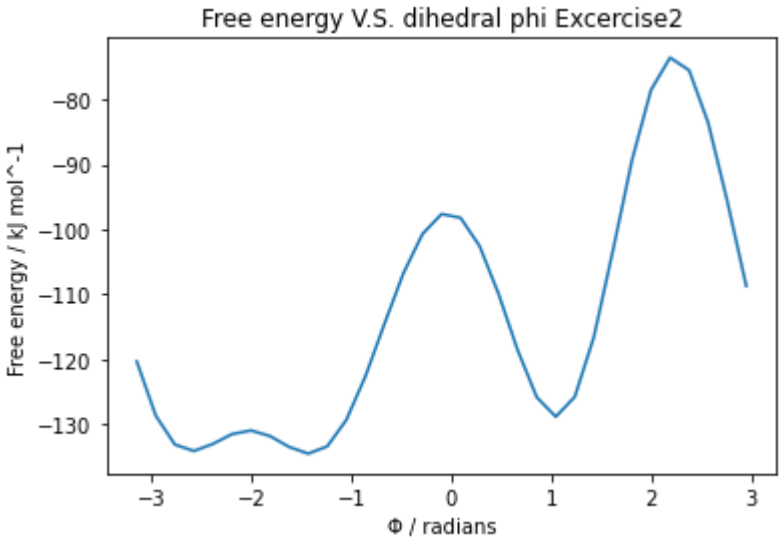
In [45]:

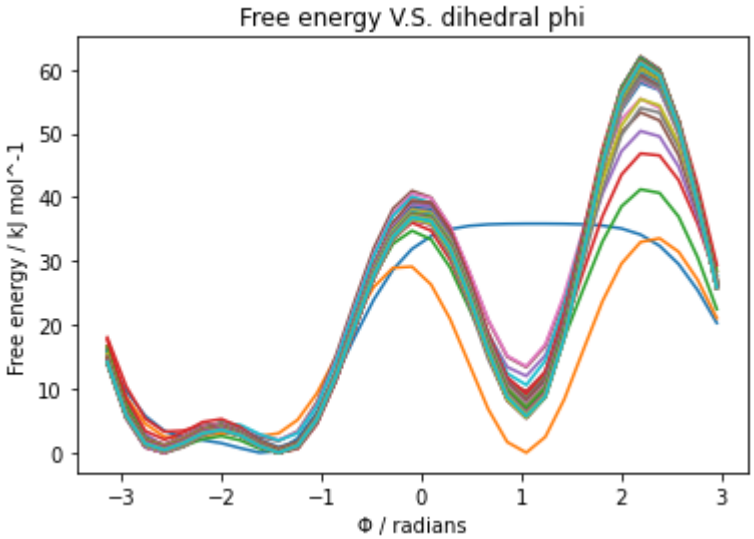
```
#Exercise 1
import pandas as pd
from matplotlib import pyplot as plt
import mdtraj as md
import numpy as np

phi, energy, unknown = np.loadtxt('COLVAR_A.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 [55]:

```
#Estimates of the free energy as a function of the dihedral phi calculated ev

import glob
from PIL import Image

for i in range(100):
    filename = f'fes_{i}.dat'
    phi, energy, unknown = np.loadtxt(filename, 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')

plt.show()
```



In [ ]: