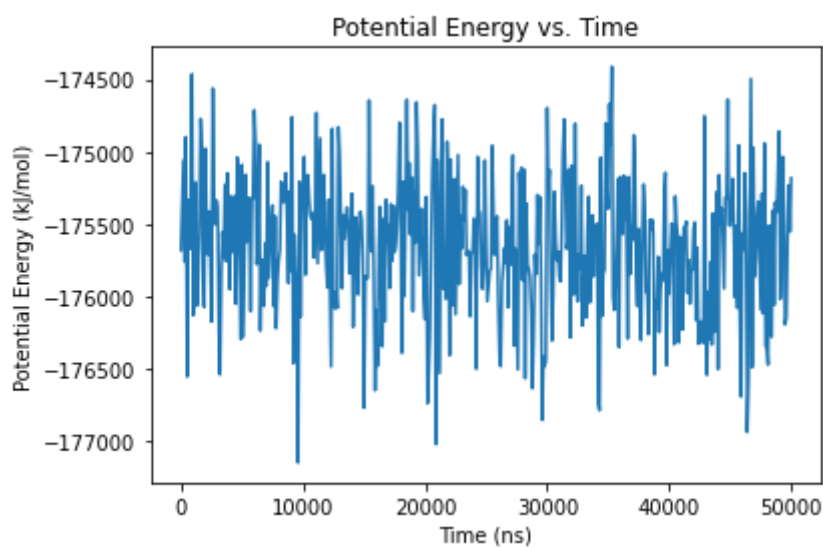


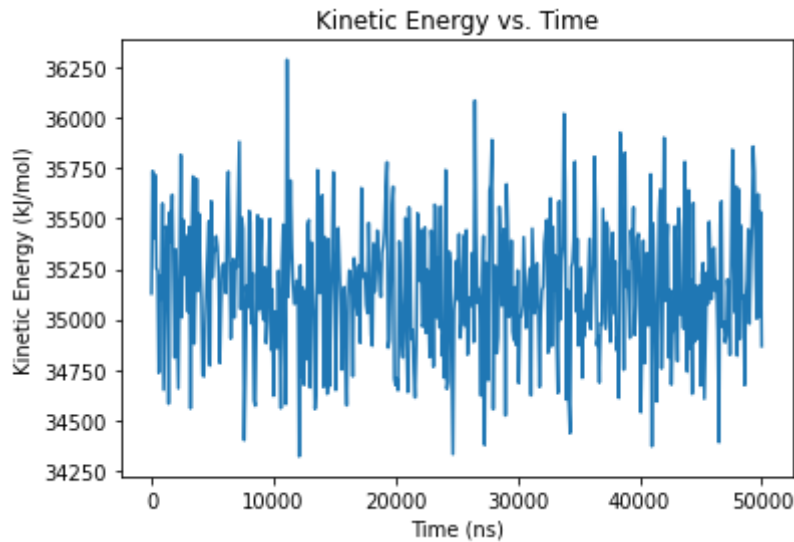
```
In [2]: # import numpy and matplotlib
import numpy as np
import matplotlib.pyplot as plt

# open .xvg file and read data from line 30
with open('1hz3_T310.run.25000000.energy.xvg') as f:
    data = f.readlines()[29:]
```

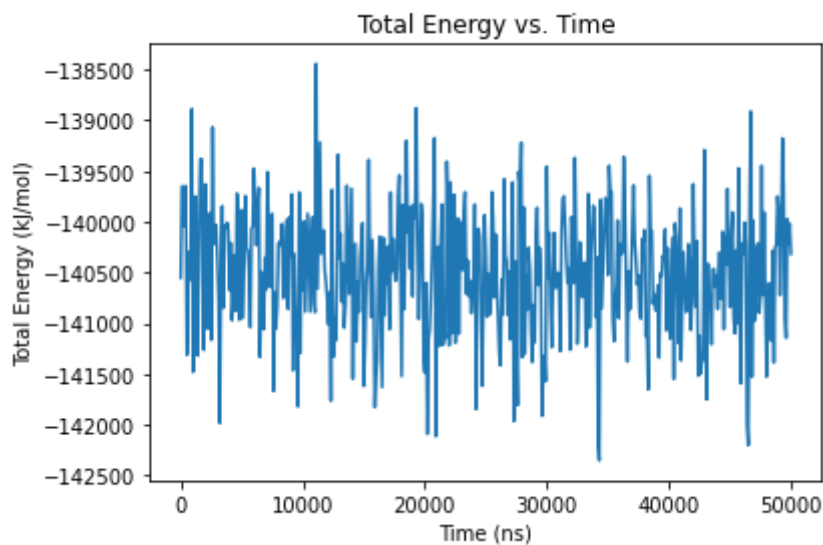
```
In [3]: # plot data from .xvg file as a function of time (ns) and Potential Energy
# title graph "Potential Energy vs. Time"
plt.plot([float(line.split()[0]) for line in data], [float(line.split()[1])])
plt.title('Potential Energy vs. Time')
plt.xlabel('Time (ns)')
plt.ylabel('Potential Energy (kJ/mol)')
plt.show()
```



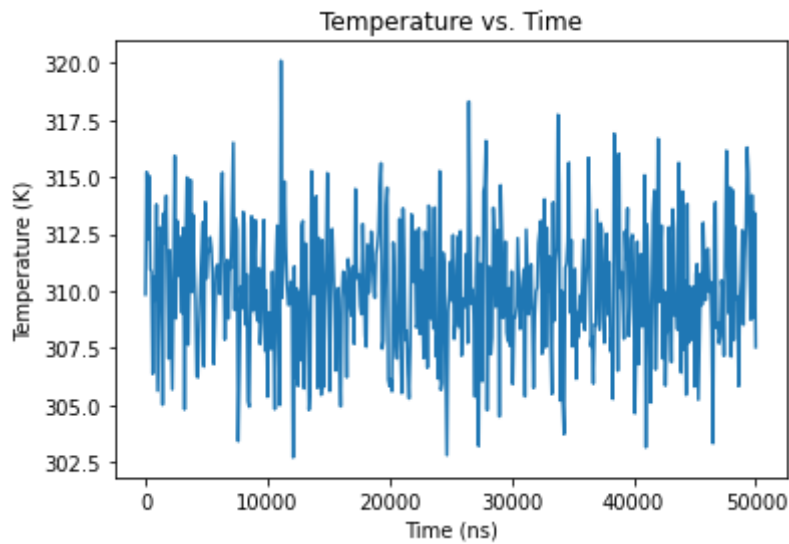
```
In [4]: # plot data from .xvg file as a function of time (ns) and Kinetic Energy (kJ/mol)
# title graph "Kinetic Energy vs. Time"
plt.plot([float(line.split()[0]) for line in data], [float(line.split()[2])])
plt.title('Kinetic Energy vs. Time')
plt.xlabel('Time (ns)')
plt.ylabel('Kinetic Energy (kJ/mol)')
plt.show()
```



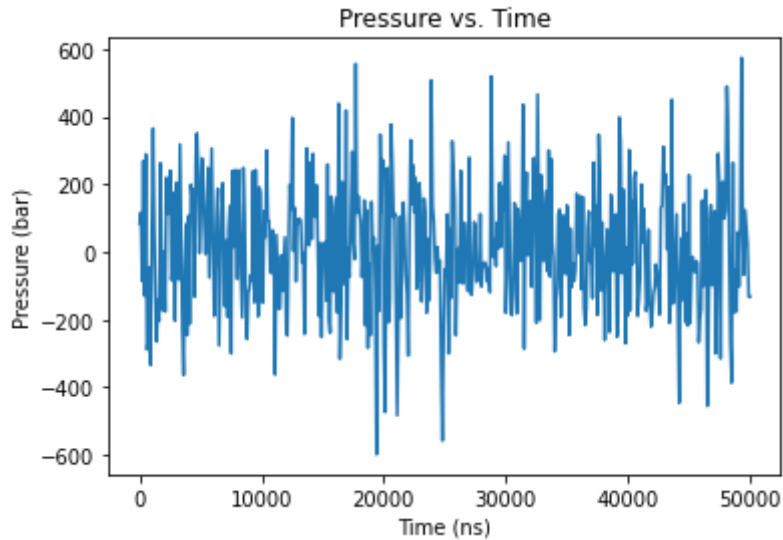
```
In [5]: # plot data from .xvg file as a function of time (ns) and Total Energy (kJ/mol)
# title graph "Total Energy vs. Time"
plt.plot([float(line.split()[0]) for line in data], [float(line.split()[3])])
plt.title('Total Energy vs. Time')
plt.xlabel('Time (ns)')
plt.ylabel('Total Energy (kJ/mol)')
plt.show()
```



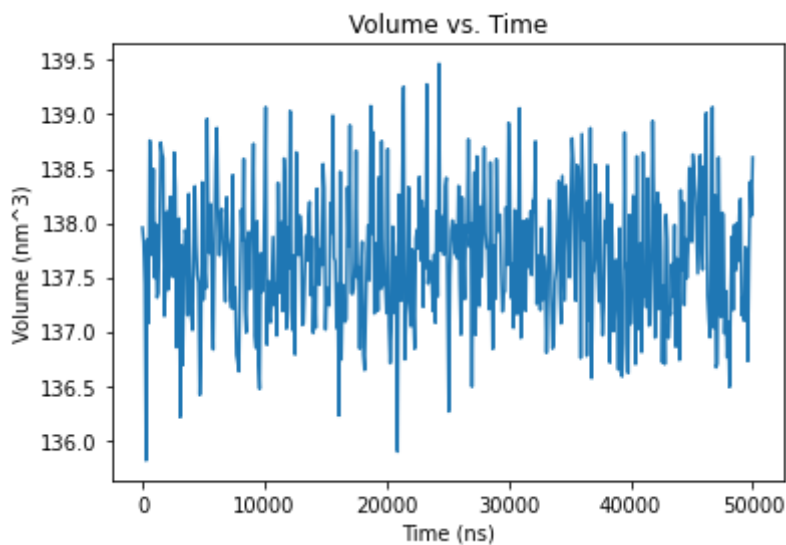
```
In [6]: # plot data from .xvg file as a function of time (ns) and Temperature (K) w
# title graph "Temperature vs. Time"
plt.plot([float(line.split()[0]) for line in data], [float(line.split()[4])])
plt.title('Temperature vs. Time')
plt.xlabel('Time (ns)')
plt.ylabel('Temperature (K)')
plt.show()
```



```
In [7]: # plot data from .xvg file as a function of time (ns) and Pressure (bar) with  
# title graph "Pressure vs. Time"  
plt.plot([float(line.split()[0]) for line in data], [float(line.split()[5])])  
plt.title('Pressure vs. Time')  
plt.xlabel('Time (ns)')  
plt.ylabel('Pressure (bar)')  
plt.show()
```



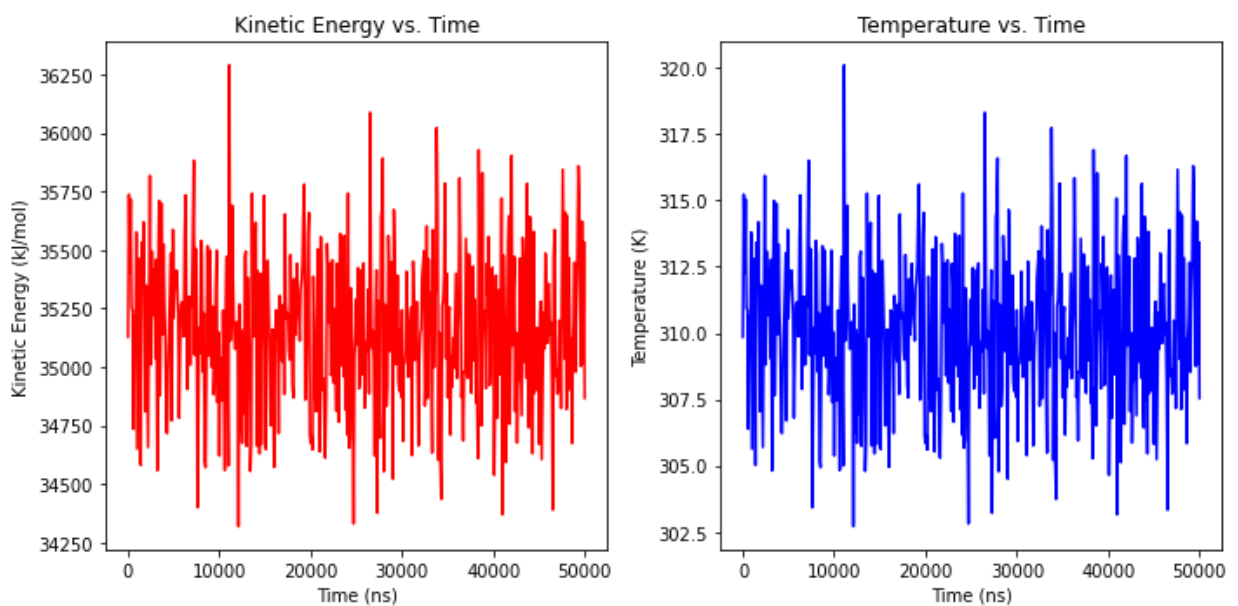
```
In [8]: # plot data from .xvg file as a function of time (ns) and Volume (nm^3) with  
# title graph "Volume vs. Time"  
plt.plot([float(line.split()[0]) for line in data], [float(line.split()[6])])  
plt.title('Volume vs. Time')  
plt.xlabel('Time (ns)')  
plt.ylabel('Volume (nm^3)')  
plt.show()
```



```

In [15]: # print out two graphs side by side with kinetic energy vs time and tempera
# make kinetic energy and temperature lines different colors
# title graphs "Kinetic Energy vs. Time" and "Temperature vs. Time"
# space graphs out so they are not on top of each other and enlarge graphs
fig, (ax1, ax2) = plt.subplots(1, 2, figsize=(10, 5))
ax1.plot([float(line.split()[0]) for line in data], [float(line.split()[2])])
ax1.set_title('Kinetic Energy vs. Time')
ax1.set_xlabel('Time (ns)')
ax1.set_ylabel('Kinetic Energy (kJ/mol)')
ax2.plot([float(line.split()[0]) for line in data], [float(line.split()[4])])
ax2.set_title('Temperature vs. Time')
ax2.set_xlabel('Time (ns)')
ax2.set_ylabel('Temperature (K)')
plt.tight_layout()
plt.show()

```



In []: