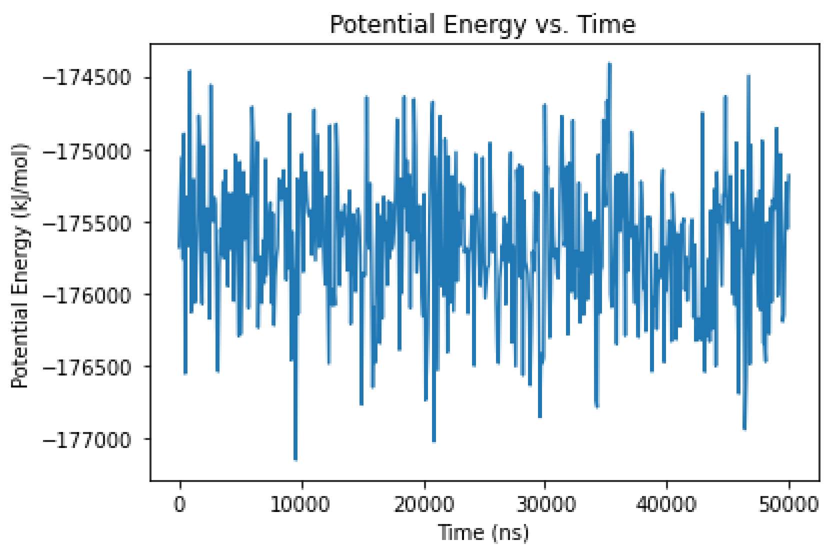
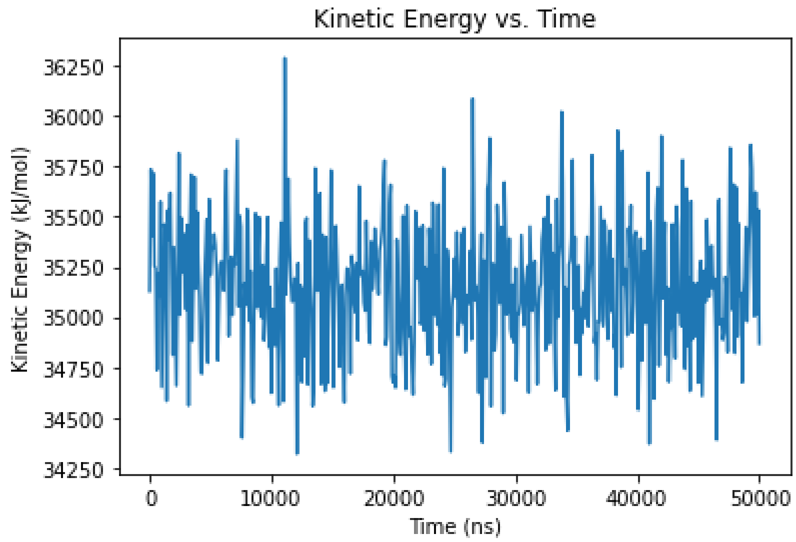
In [2]:
```
# import numpy and matplotlib
import numpy as np
import matplotlib.pyplot as plt

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

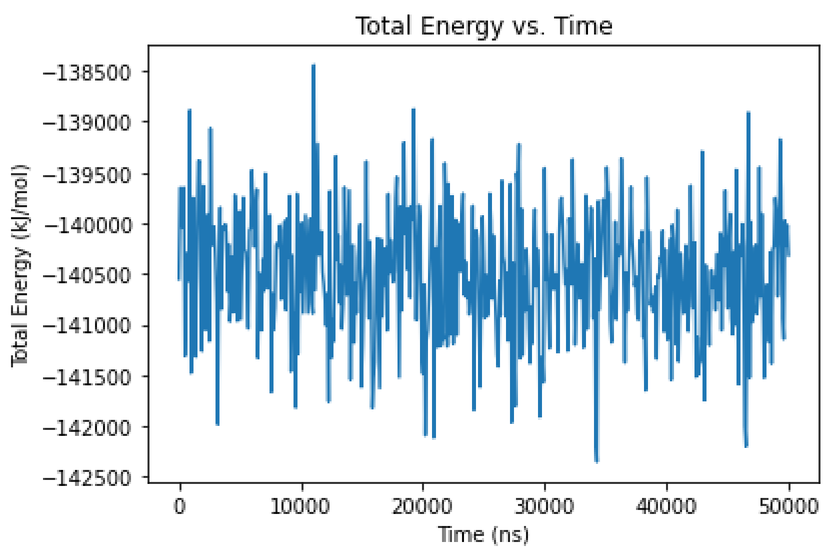
In [3]:
```
# plot data from .xvg file as a function of time (ns) and Potential Energy
# title graph "Potential Energy vs. Time"
plt.plot([float(line.split()[0]) for line in data], [float(line.split()[1])
plt.title('Potential Energy vs. Time')
plt.xlabel('Time (ns)')
plt.ylabel('Potential Energy (kJ/mol)')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



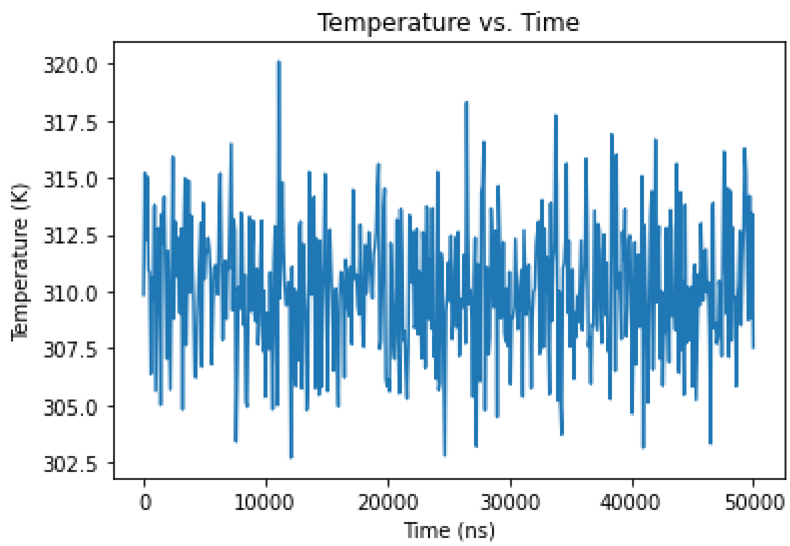
In [4]:
```
# plot data from .xvg file as a function of time (ns) and Kinetic Energy (k
# title graph "Kinetic Energy vs. Time"
plt.plot([float(line.split()[0]) for line in data], [float(line.split()[2])
plt.title('Kinetic Energy vs. Time')
plt.xlabel('Time (ns)')
plt.ylabel('Kinetic Energy (kJ/mol)')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



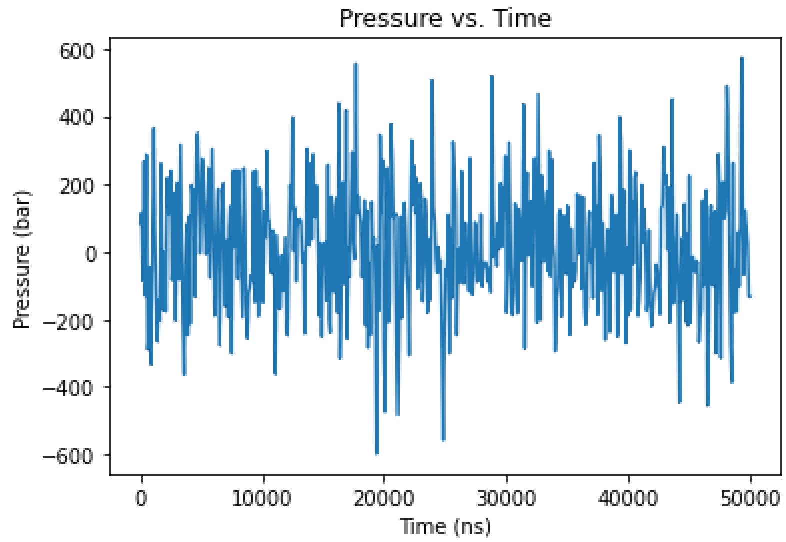

In [5]:
```
# plot data from .xvg file as a function of time (ns) and Total Energy (kJ/
# title graph "Total Energy vs. Time"
plt.plot([float(line.split()[0]) for line in data], [float(line.split()[3])
plt.title('Total Energy vs. Time')
plt.xlabel('Time (ns)')
plt.ylabel('Total Energy (kJ/mol)')
plt.show()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



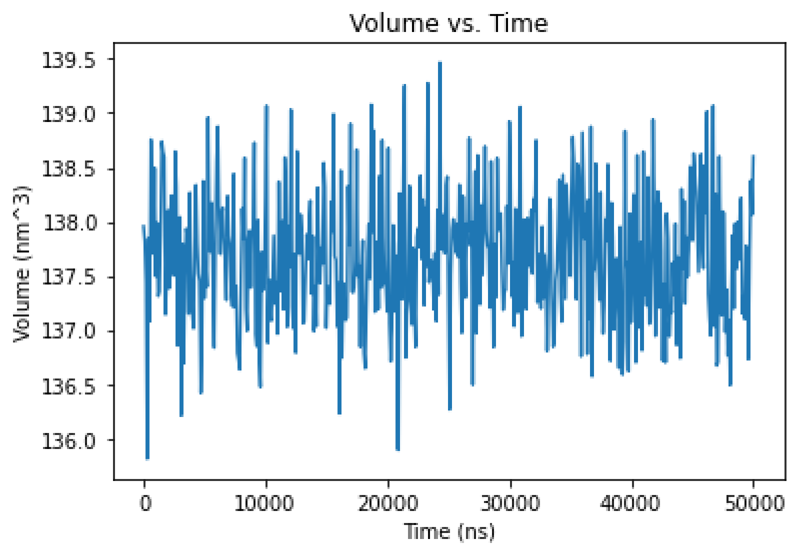
In [6]:
```
# plot data from .xvg file as a function of time (ns) and Temperature (K) w
# title graph "Temperature vs. Time"
plt.plot([float(line.split()[0]) for line in data], [float(line.split()[4])
plt.title('Temperature vs. Time')
plt.xlabel('Time (ns)')
plt.ylabel('Temperature (K)')
plt.show()
```



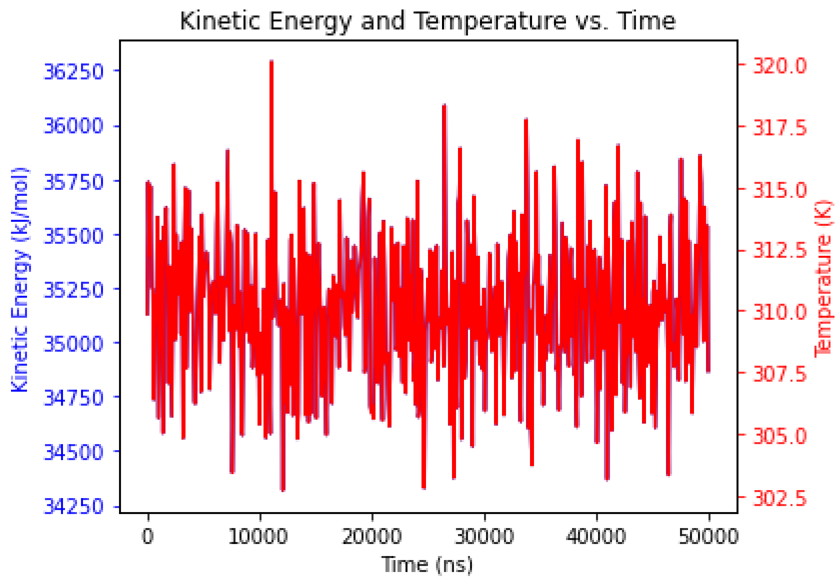
In [7]:
```
# plot data from .xvg file as a function of time (ns) and Pressure (bar) wi
# title graph "Pressure vs. Time"
plt.plot([float(line.split()[0]) for line in data], [float(line.split()[5])
plt.title('Pressure vs. Time')
plt.xlabel('Time (ns)')
plt.ylabel('Pressure (bar)')
plt.show()
```




In [8]:
```
# plot data from .xvg file as a function of time (ns) and Volume (nm^3) wit
# 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 [11]:
```
# plot kinetic energy and temperature at y axis and time at x axis and scal
# title graph "Kinetic Energy and Temperature vs. Time"
fig, ax1 = plt.subplots()
ax1.plot([float(line.split()[0]) for line in data], [float(line.split()[2])
ax1.set_xlabel('Time (ns)')
ax1.set_ylabel('Kinetic Energy (kJ/mol)', color='b')
ax1.tick_params('y', colors='b')
ax2 = ax1.twinx()
ax2.plot([float(line.split()[0]) for line in data], [float(line.split()[4])
ax2.set_ylabel('Temperature (K)', color='r')
ax2.tick_params('y', colors='r')
fig.tight_layout()
plt.title('Kinetic Energy and Temperature vs. Time')
plt.show()
```




In [ ]: