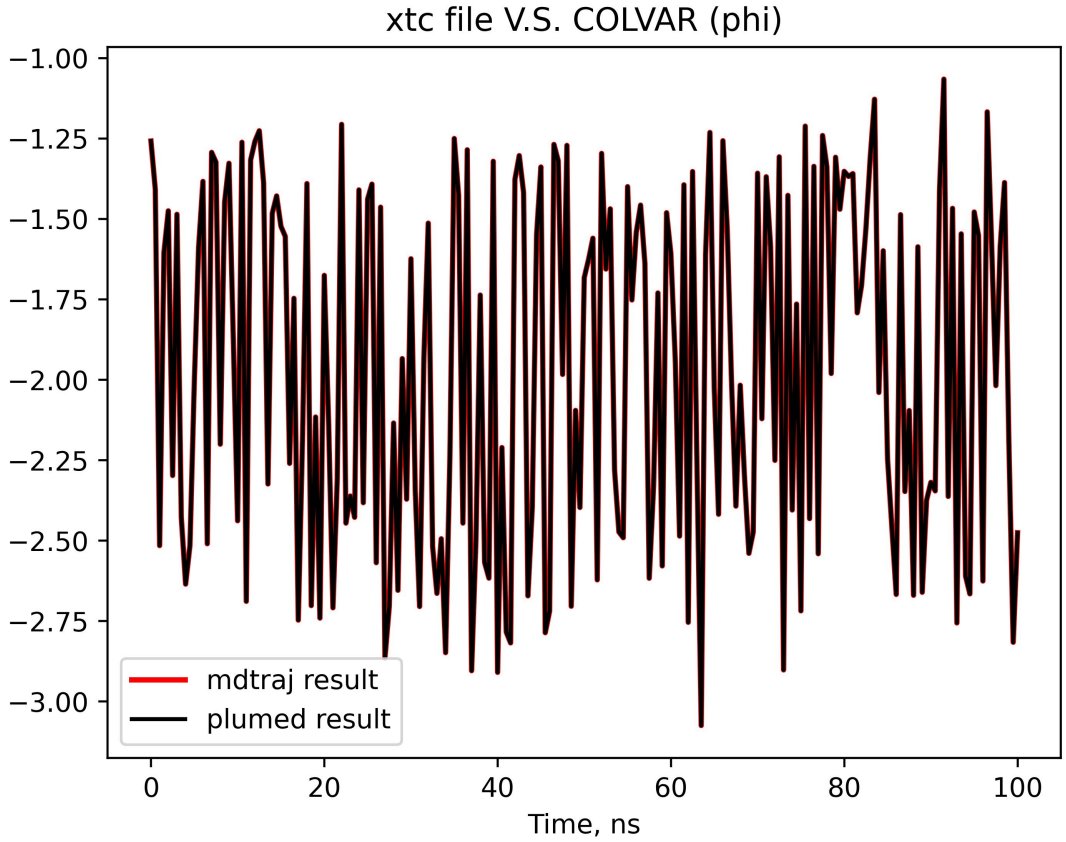
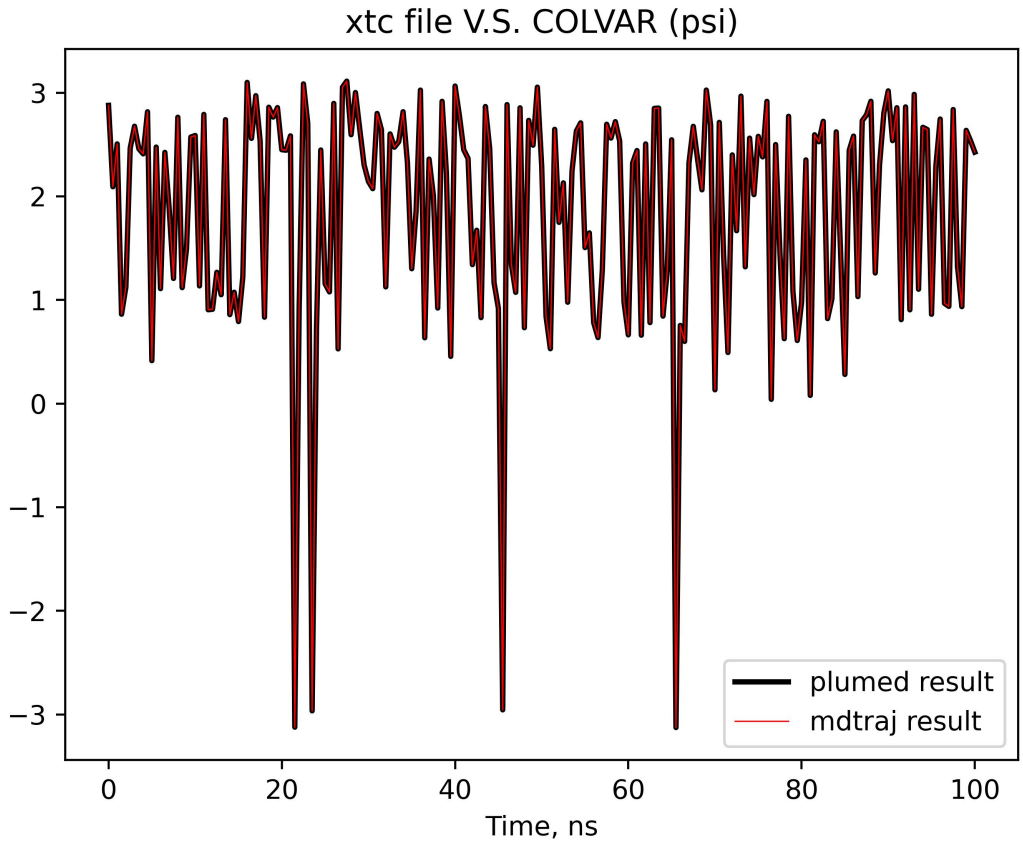
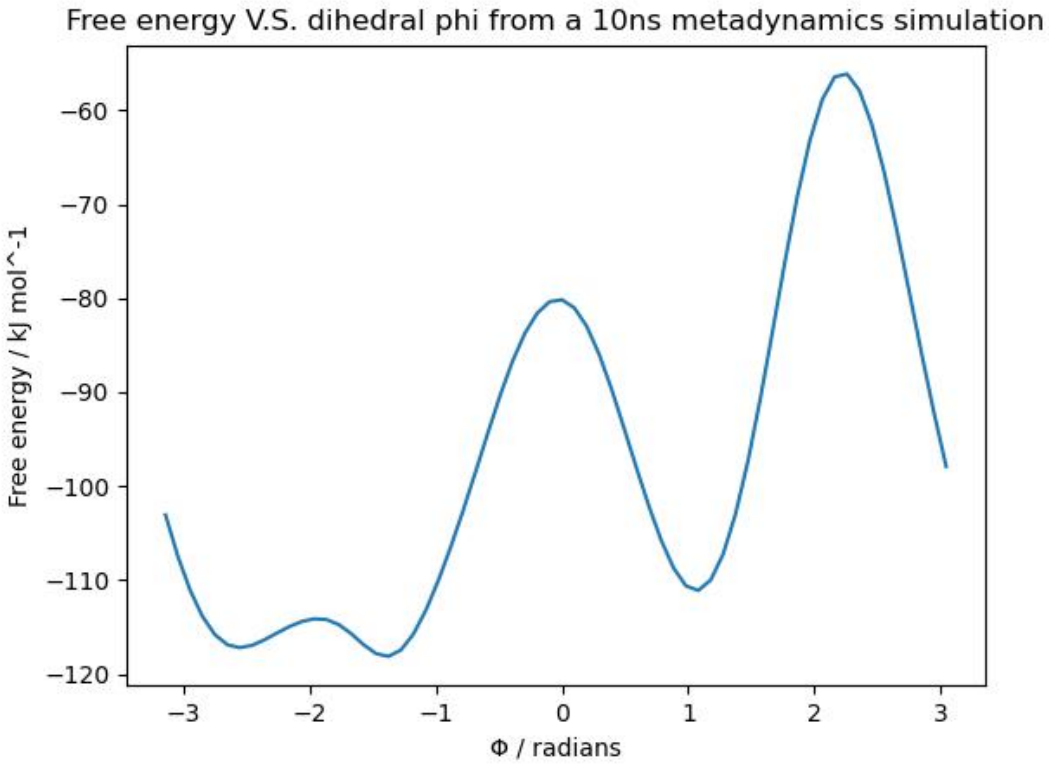
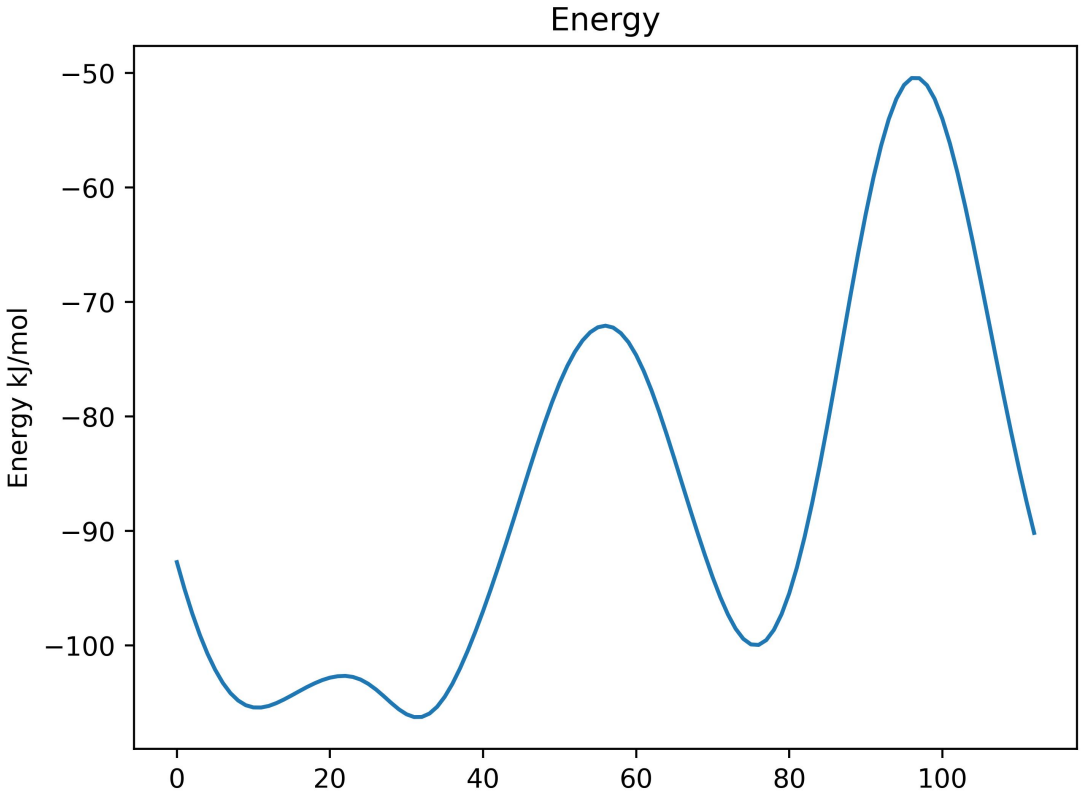
Part 2:


xtc file V.S. COLVAR (phi)
−1.00
−1.25
−1.50
−1.75
−2.00
−2.25
−2.50
−2.75
−3.00
mdtraj result
plumed result
0
20
40
60
80
100
Time, ns

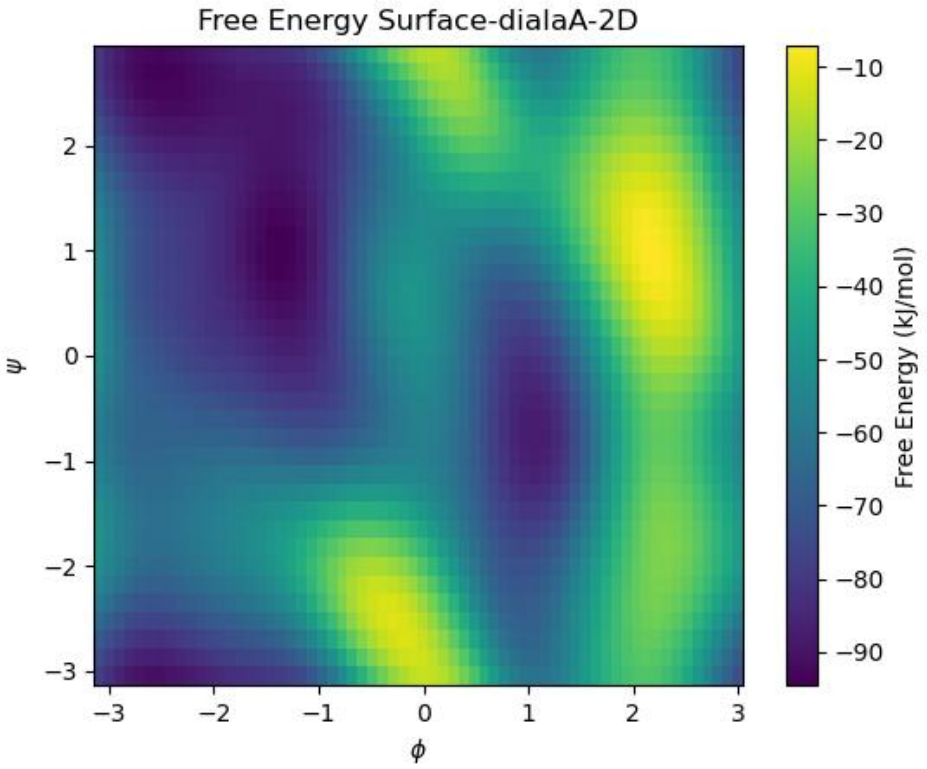

xtc file V.S. COLVAR (psi)
3
2
1
0
−1
−2
−3
plumed result
mdtraj result
0
20
40
60
80
100
Time, ns

Part 3:


Free energy V.S. dihedral phi from a 10ns metadynamics simulation
Free energy / kJ mol^-1
−60
−70
−80
−90
−100
−110
−120
−3
−2
−1
0
1
2
3
Φ / radians


Energy
Energy kJ/mol
−50
−60
−70
−80
−90
−100
0
20
40
60
80
100

Part 6:


Free Energy Surface-dialaA-2D
ψ
ϕ
Free Energy (kJ/mol)
−10
−20
−30
−40
−50
−60
−70
−80
−90
2
1
0
−1
−2
−3
−3
−2
−1
0
1
2
3