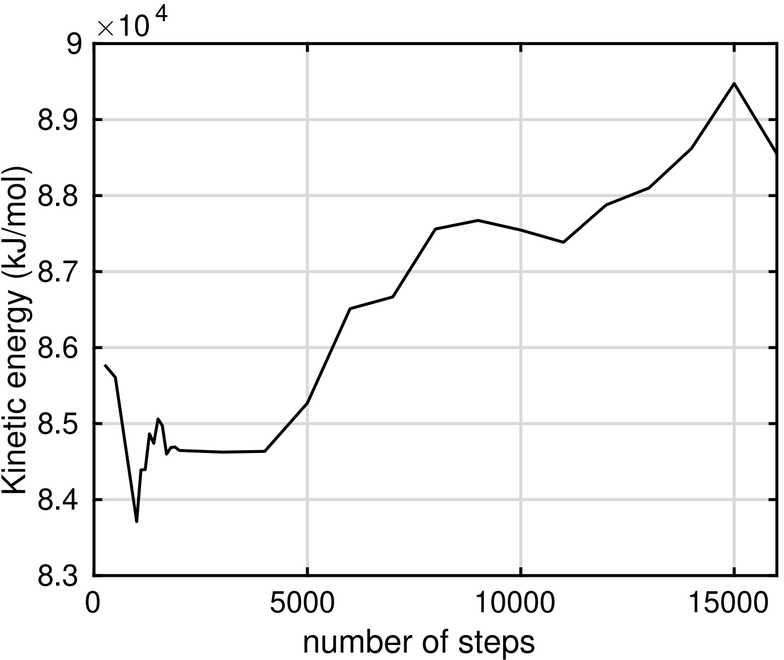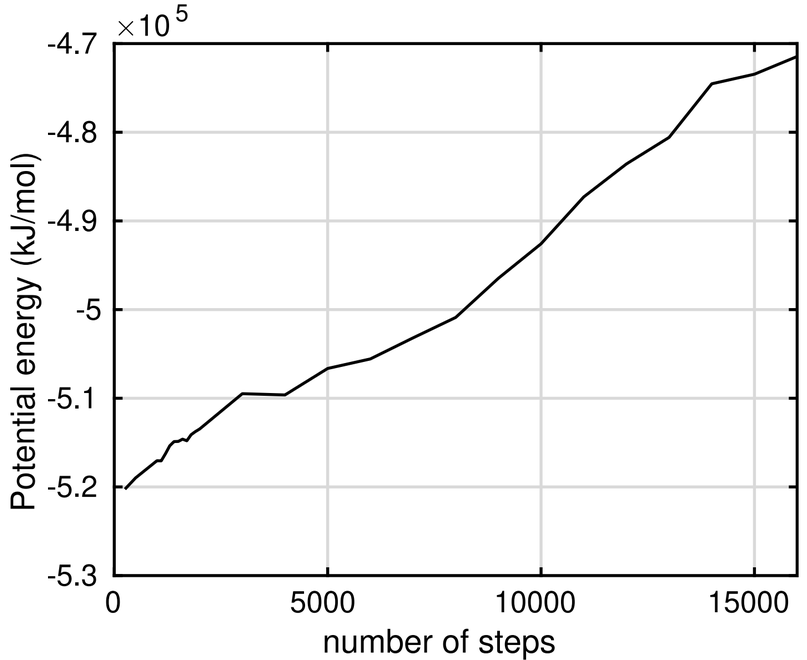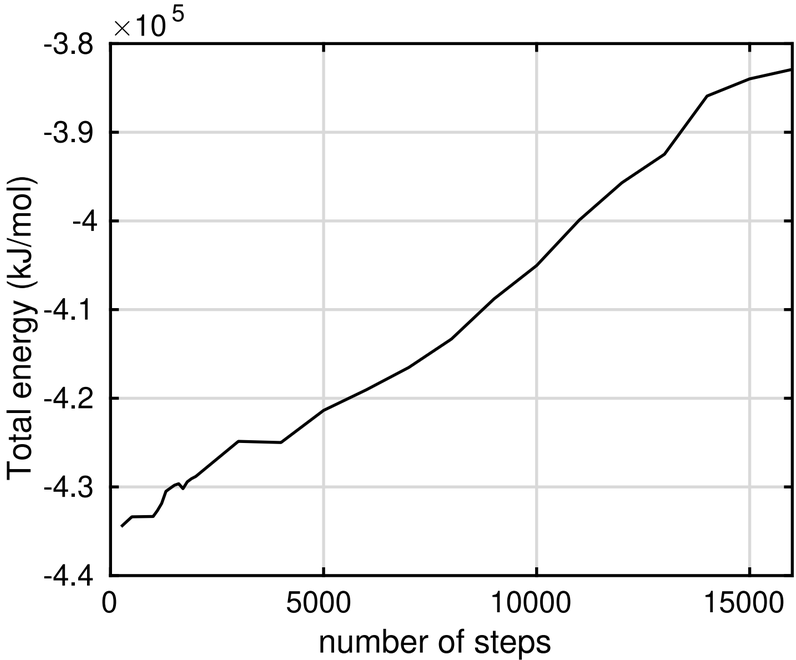Forcefield = charmm36 constraint tolerance = 1.00e-04