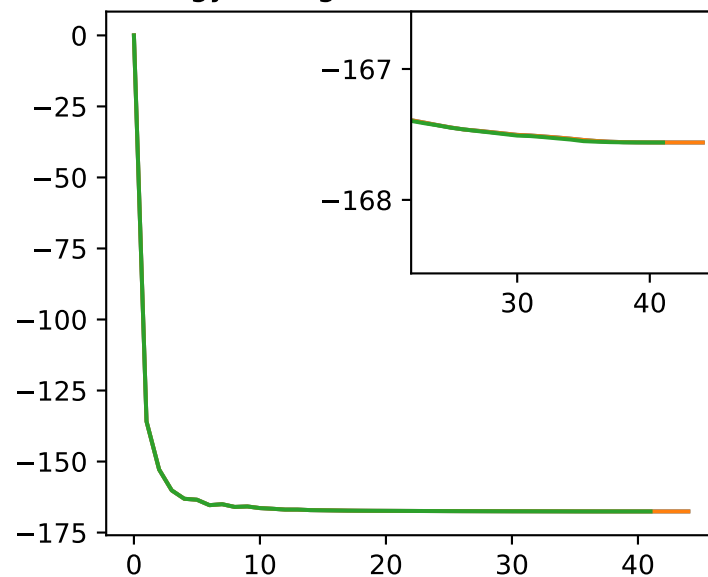
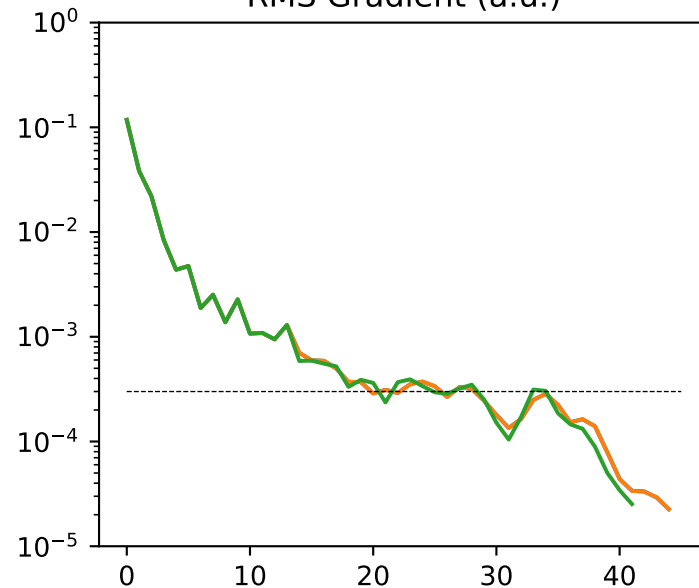


# Optimization performance for calicheamicin

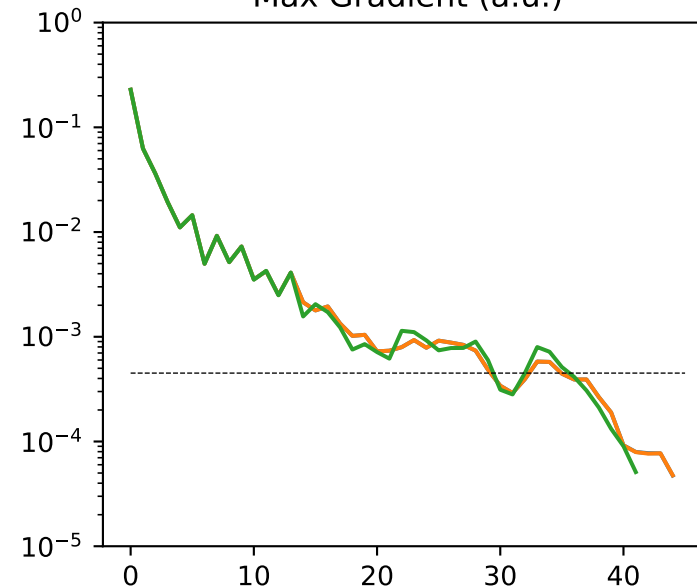
Energy change, from start (kcal/mol)



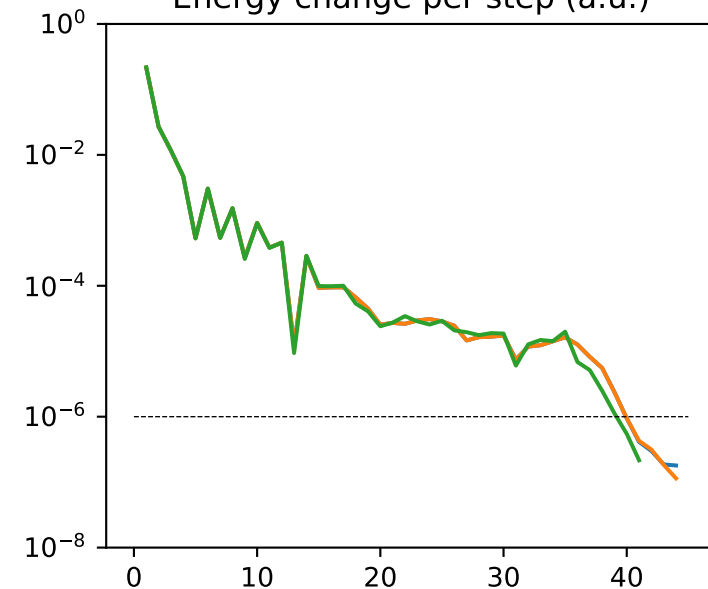
RMS Gradient (a.u.)



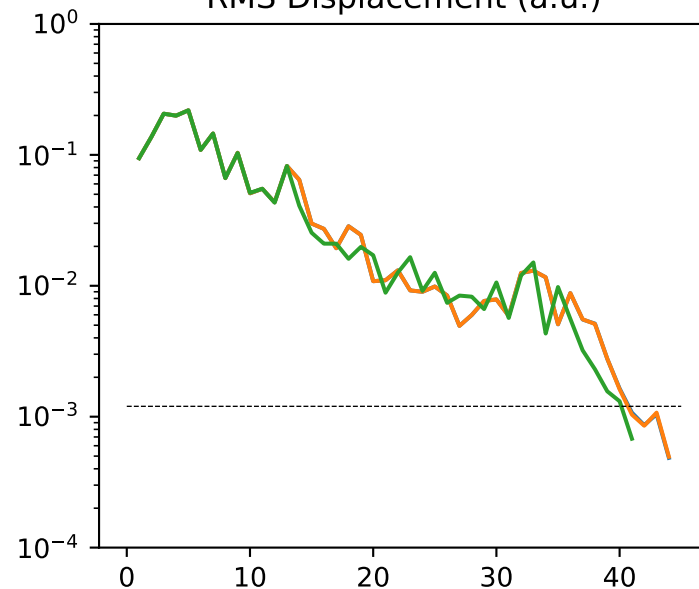
Max Gradient (a.u.)



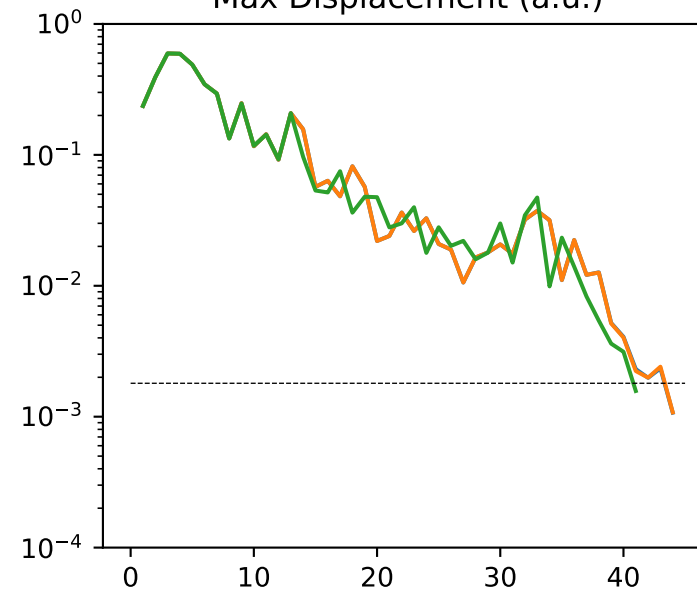
Energy change per step (a.u.)



RMS Displacement (a.u.)



Max Displacement (a.u.)



Optimization Cycle

