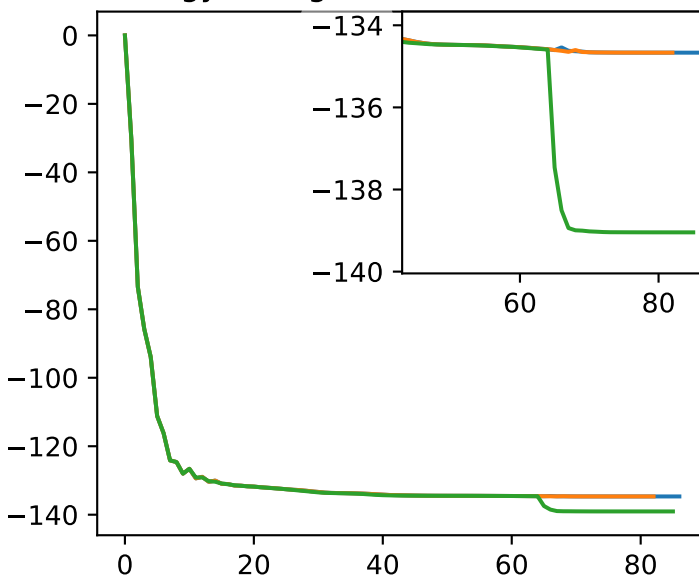
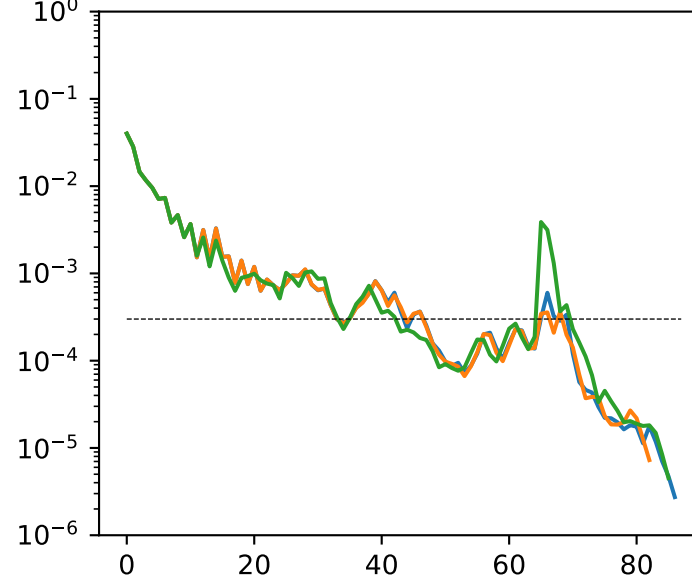


Optimization performance for heme

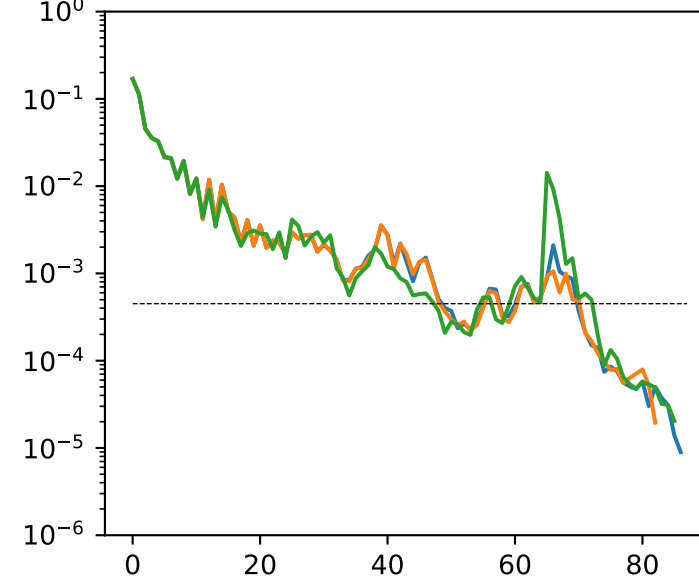
Energy change, from start (kcal/mol)



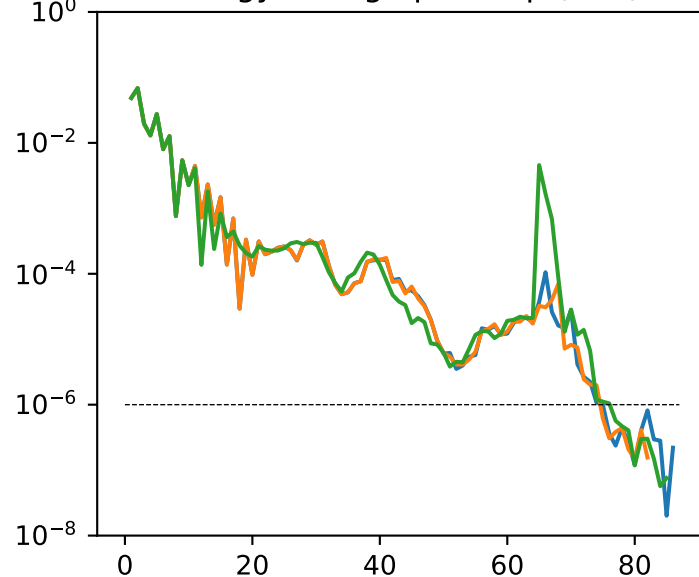
RMS Gradient (a.u.)



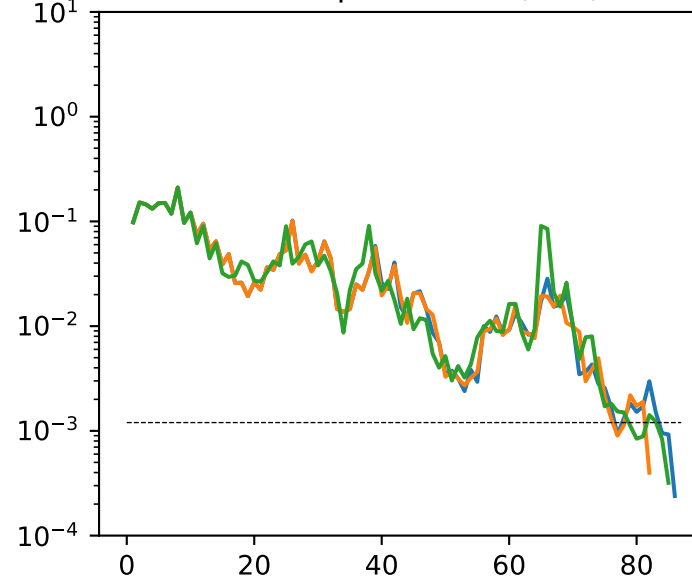
Max Gradient (a.u.)



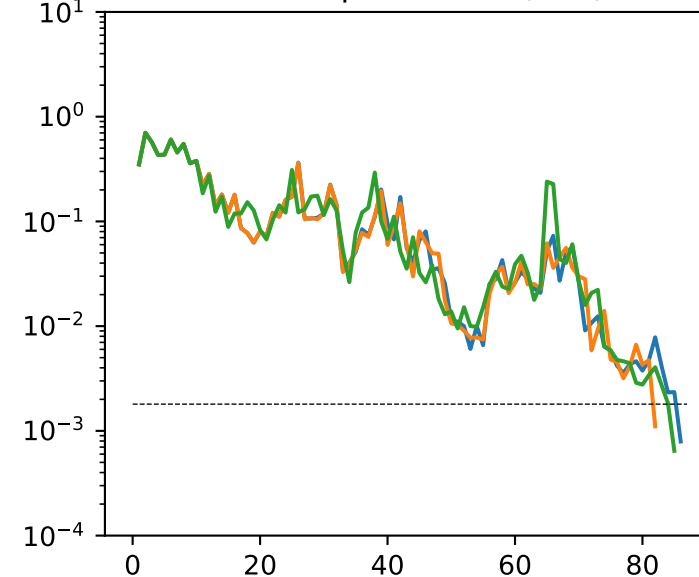
Energy change per step (a.u.)



RMS Displacement (a.u.)



Max Displacement (a.u.)



Optimization Cycle

0.8.2 Converged N=86 1.0 Converged N=85
0.9.7.2 Converged N=82