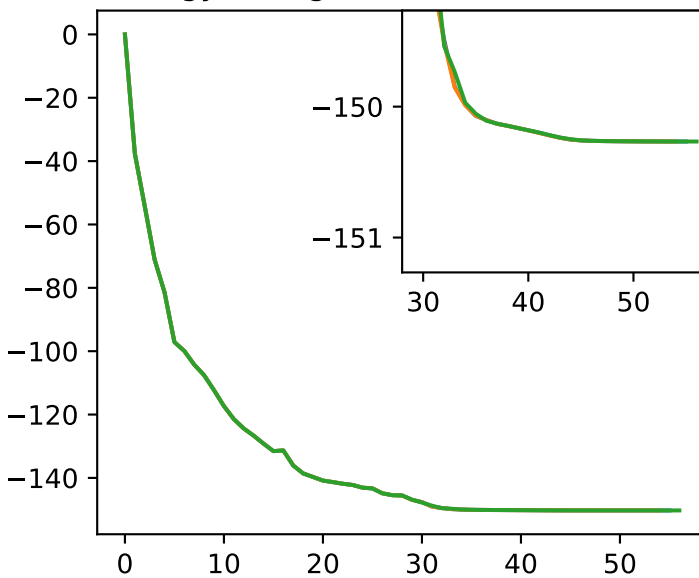
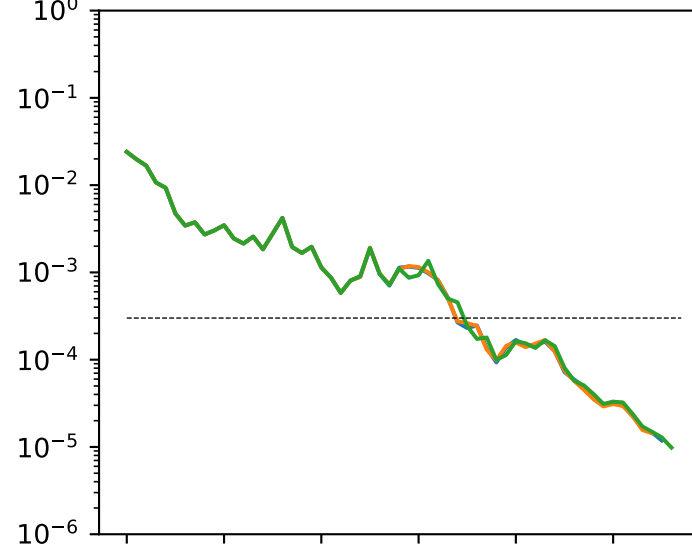


Optimization performance for azithromycin

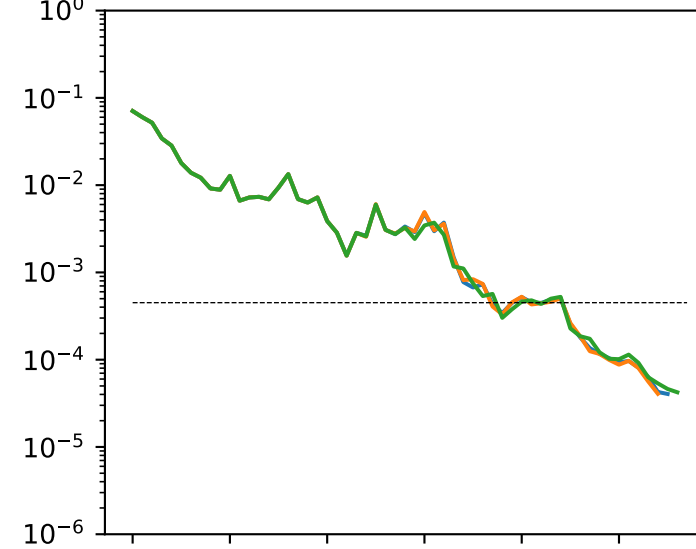
Energy change, from start (kcal/mol)



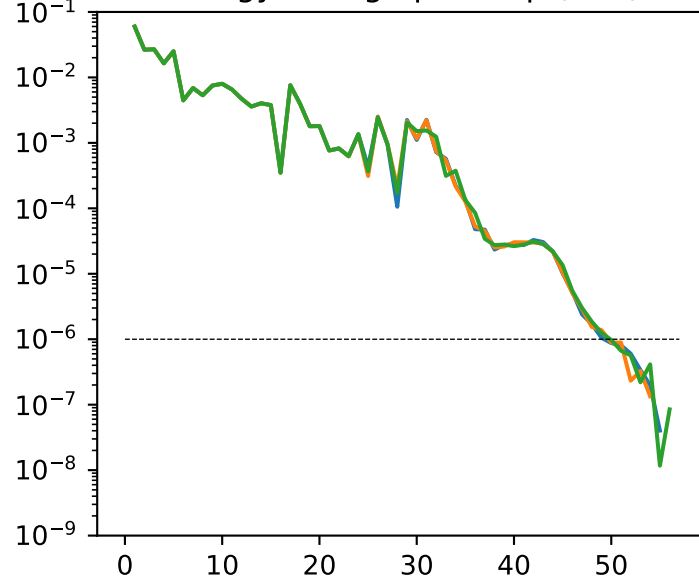
RMS Gradient (a.u.)



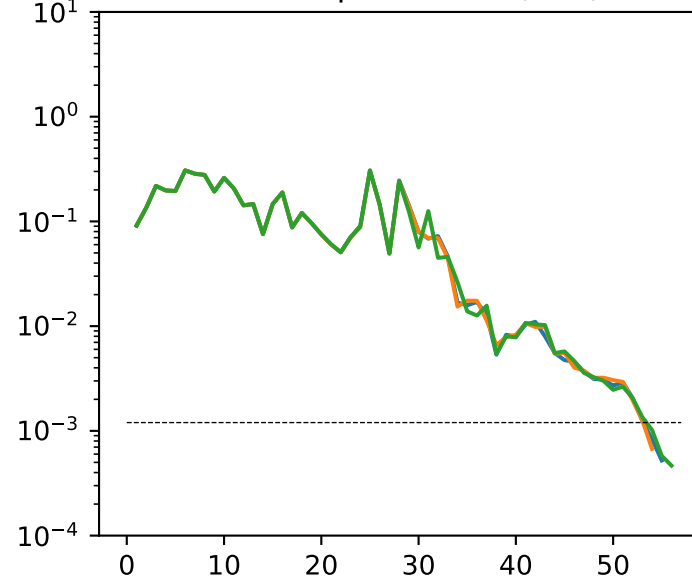
Max Gradient (a.u.)



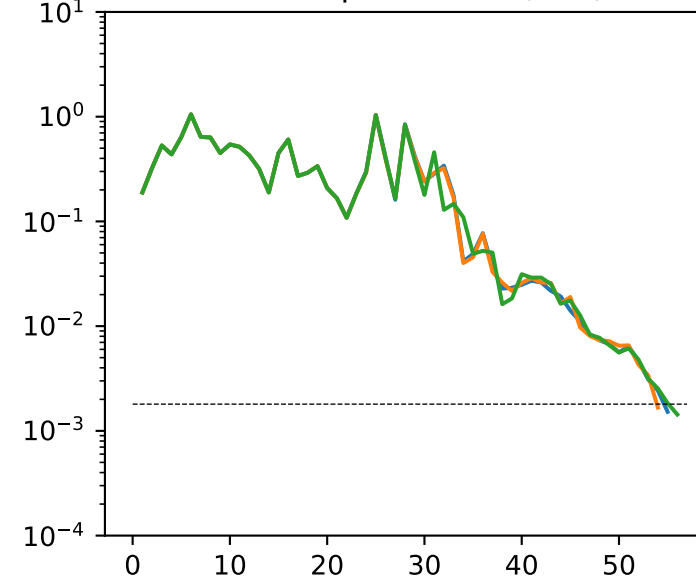
Energy change per step (a.u.)



RMS Displacement (a.u.)



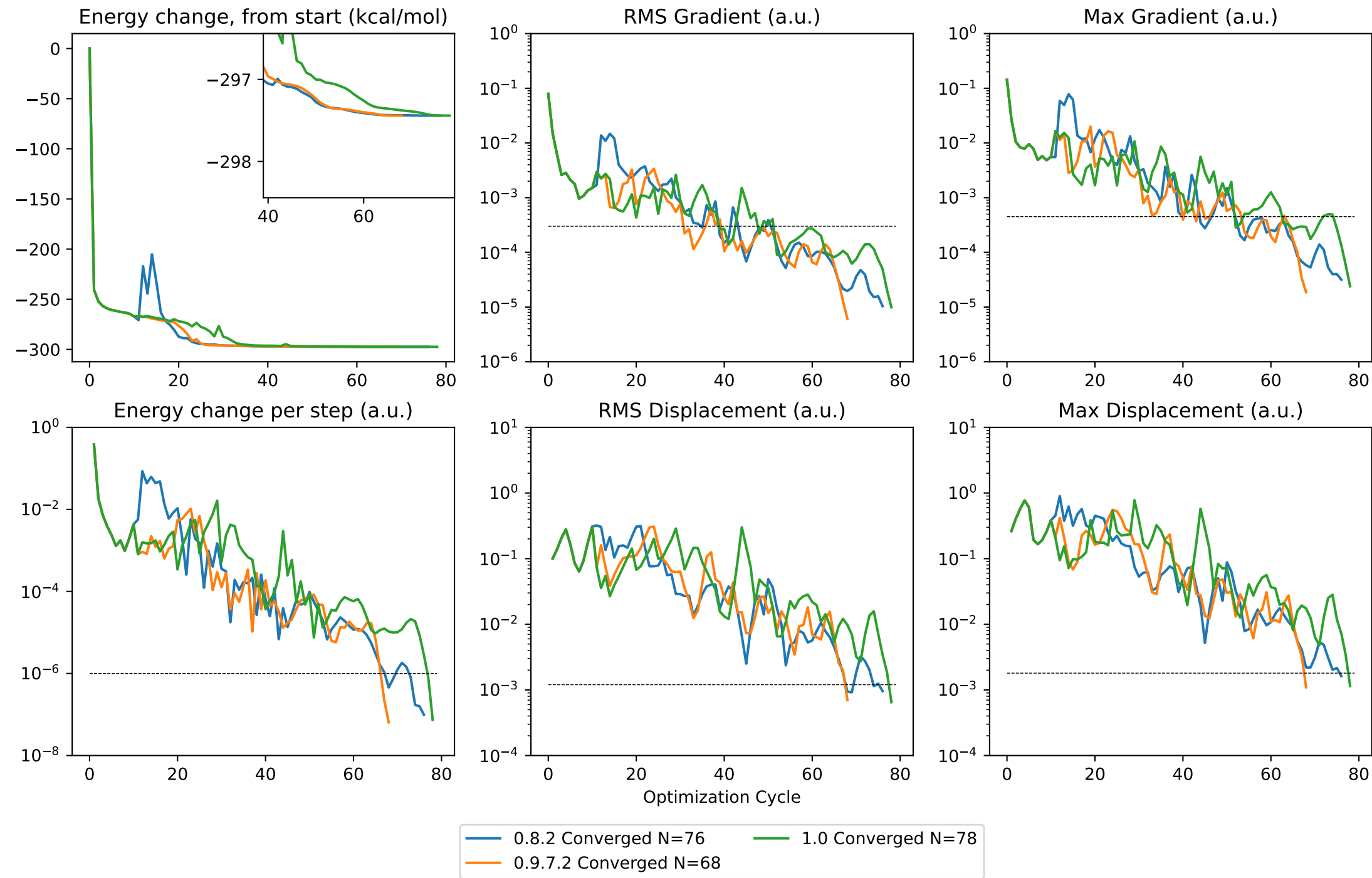
Max Displacement (a.u.)



Optimization Cycle

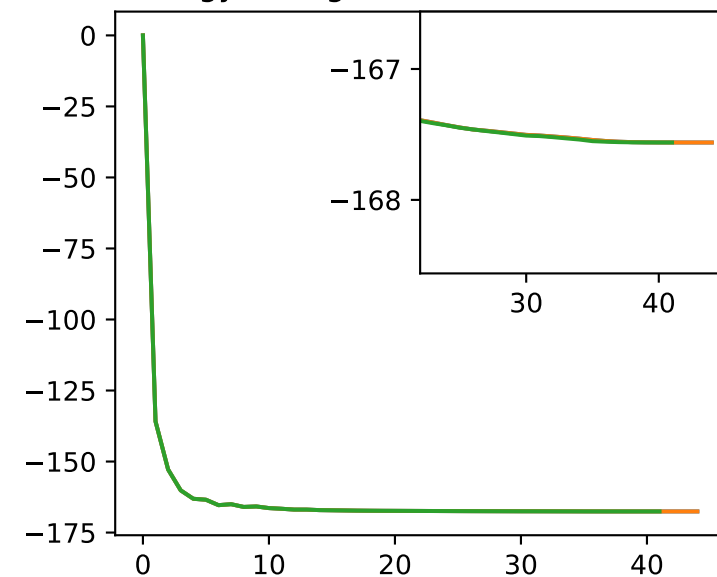
0.8.2 Converged N=55 1.0 Converged N=56
0.9.7.2 Converged N=54

Optimization performance for bucky_catcher

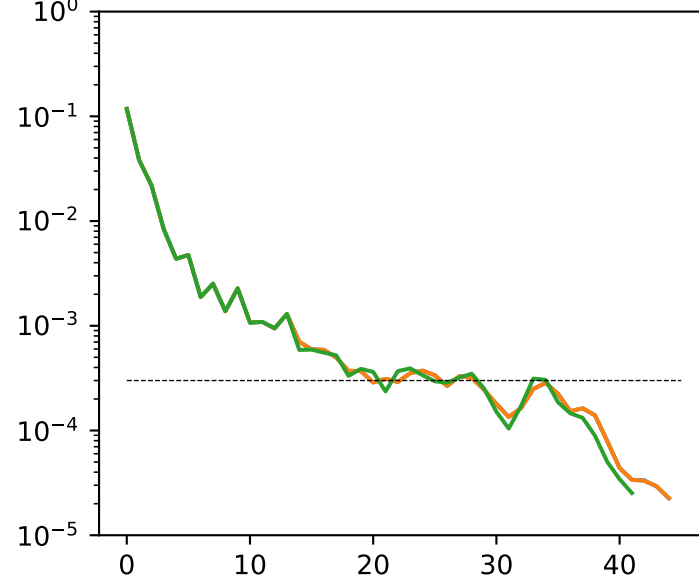


Optimization performance for calicheamicin

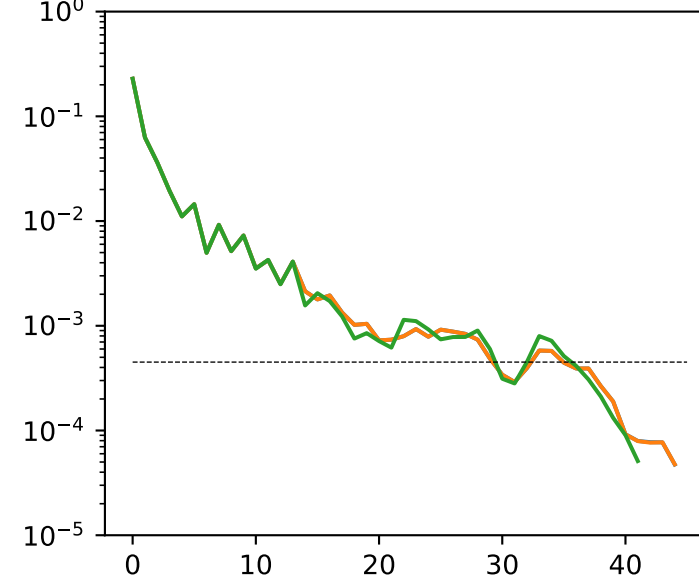
Energy change, from start (kcal/mol)



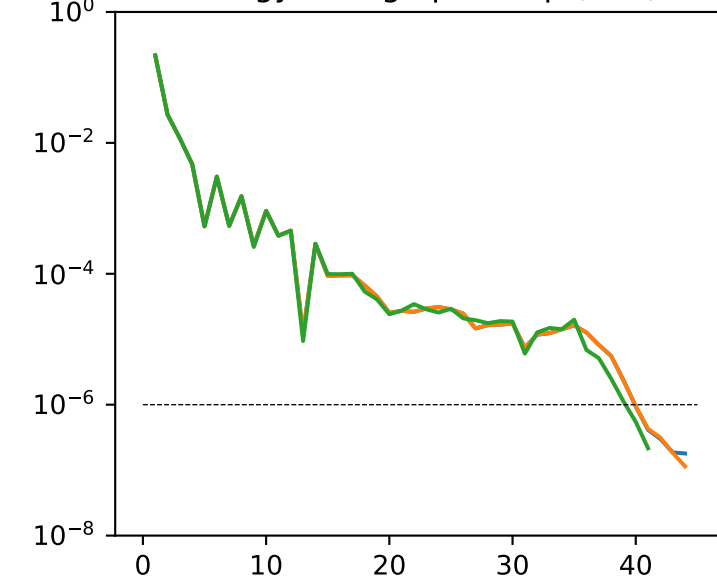
RMS Gradient (a.u.)



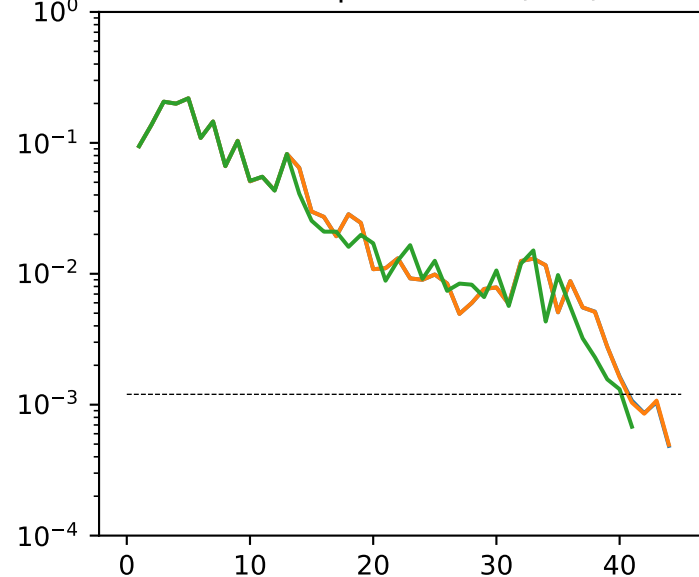
Max Gradient (a.u.)



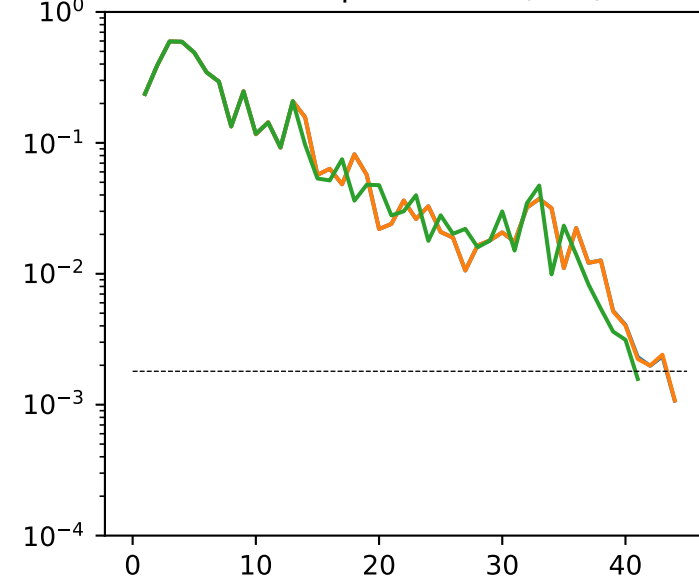
Energy change per step (a.u.)



RMS Displacement (a.u.)

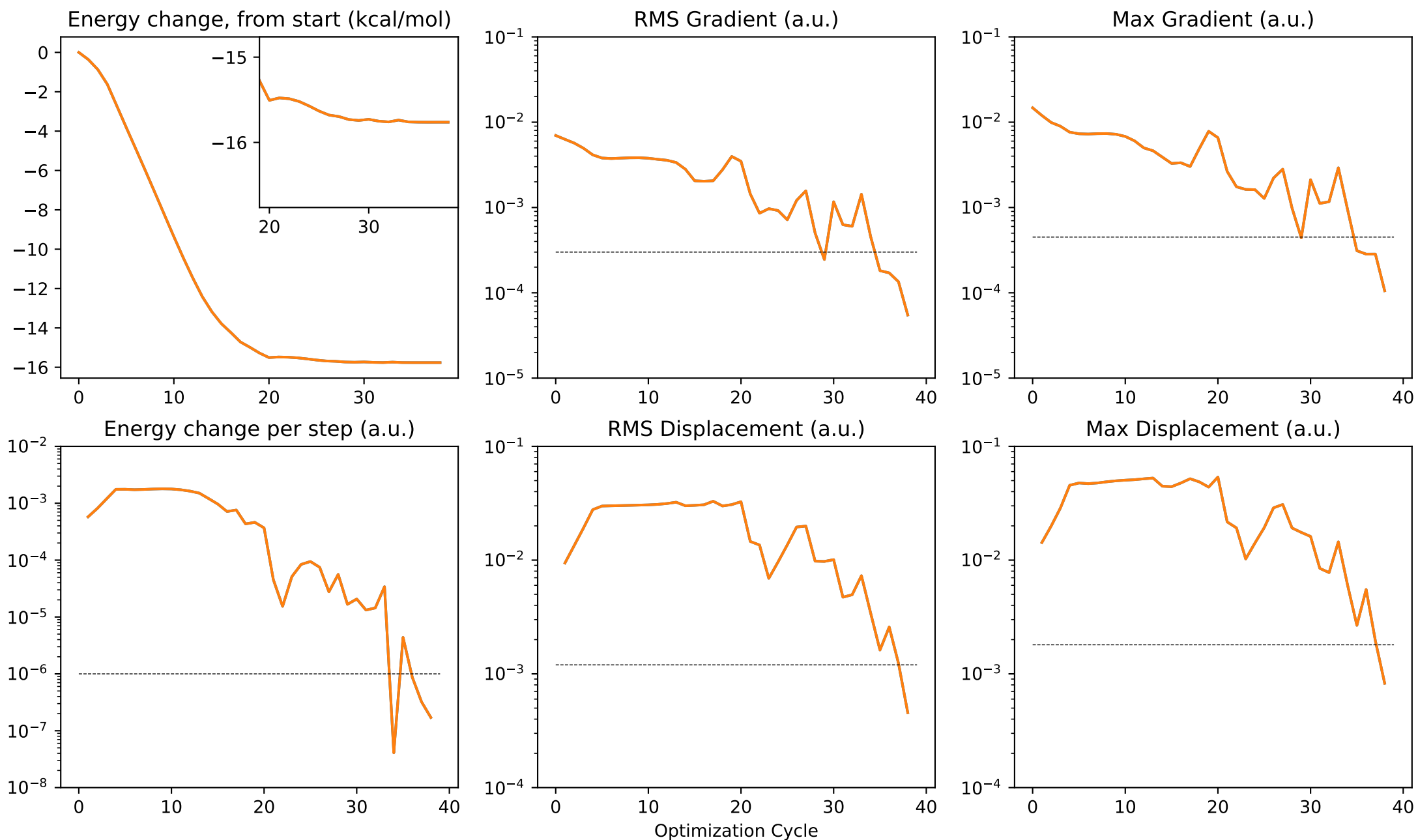


Max Displacement (a.u.)



0.8.2 Converged N=44 1.0 Converged N=41
0.9.7.2 Converged N=44

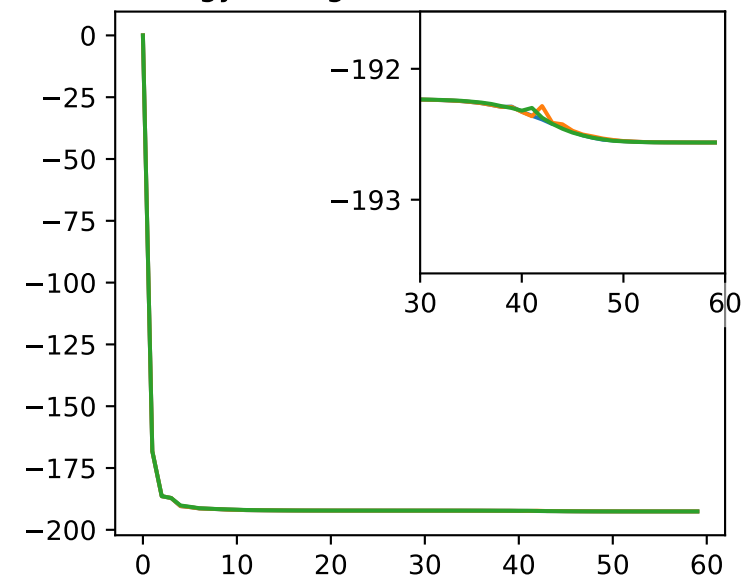
Optimization performance for carbene-ts



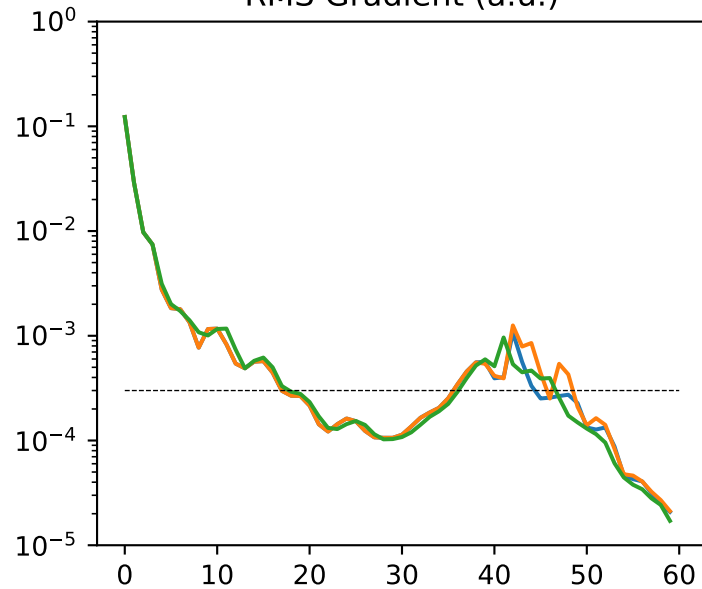
2022-07-17 Converged N=38 v1.0 Converged N=38

Optimization performance for cu-i-carborane

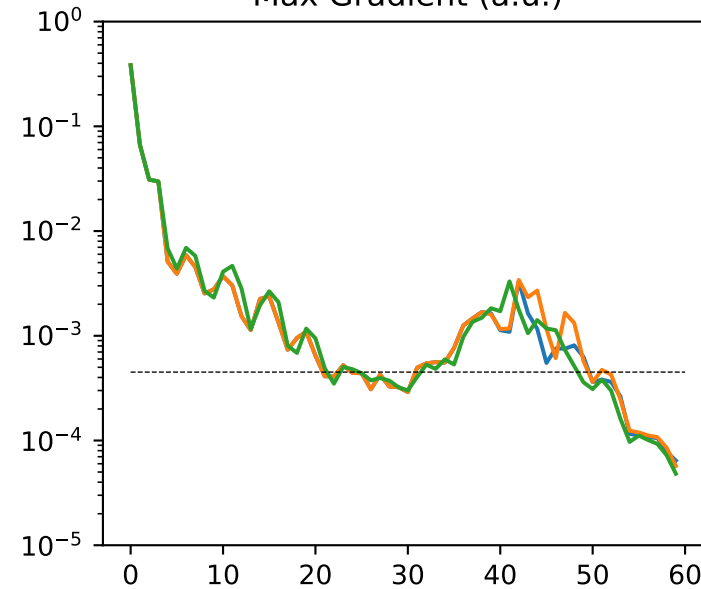
Energy change, from start (kcal/mol)



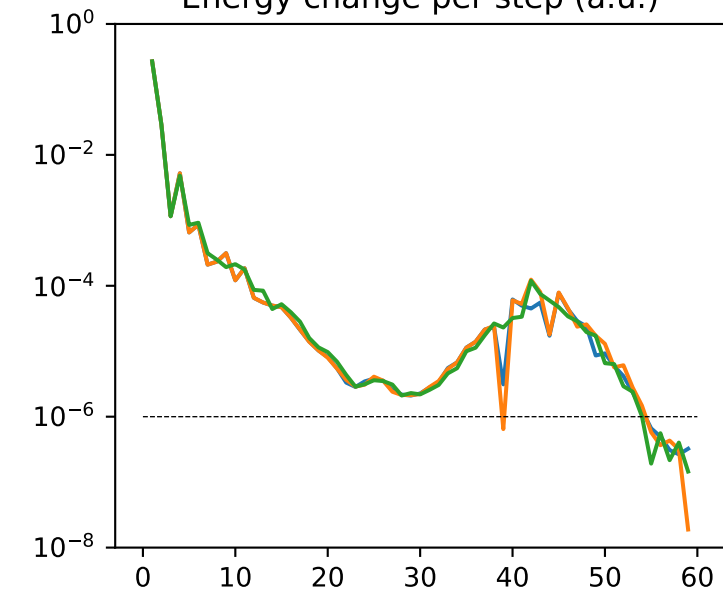
RMS Gradient (a.u.)



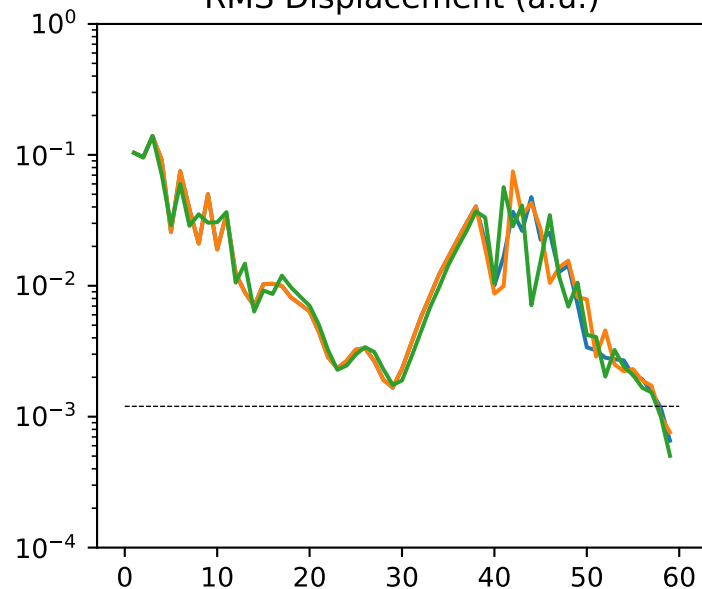
Max Gradient (a.u.)



Energy change per step (a.u.)



RMS Displacement (a.u.)

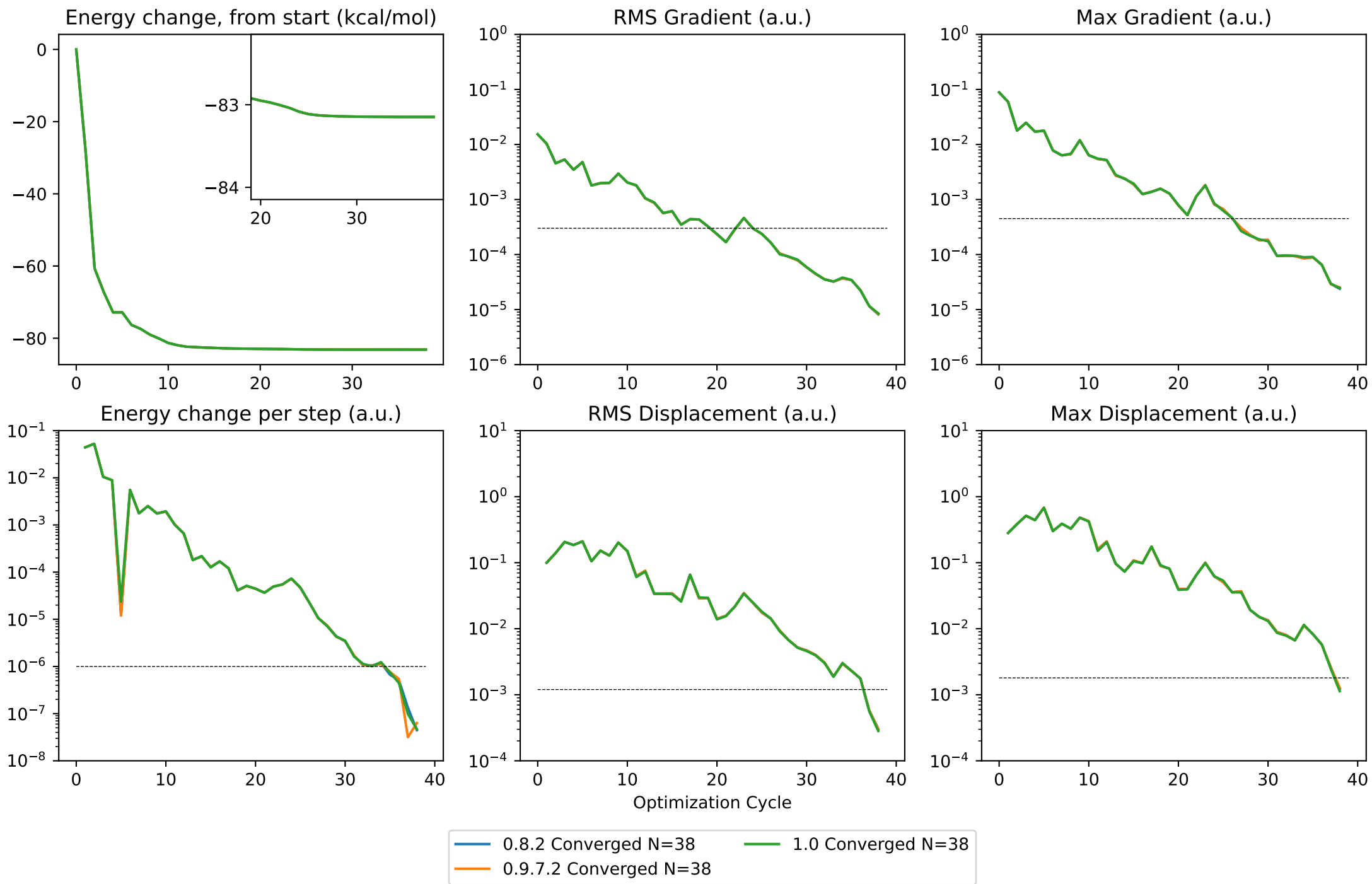


Max Displacement (a.u.)

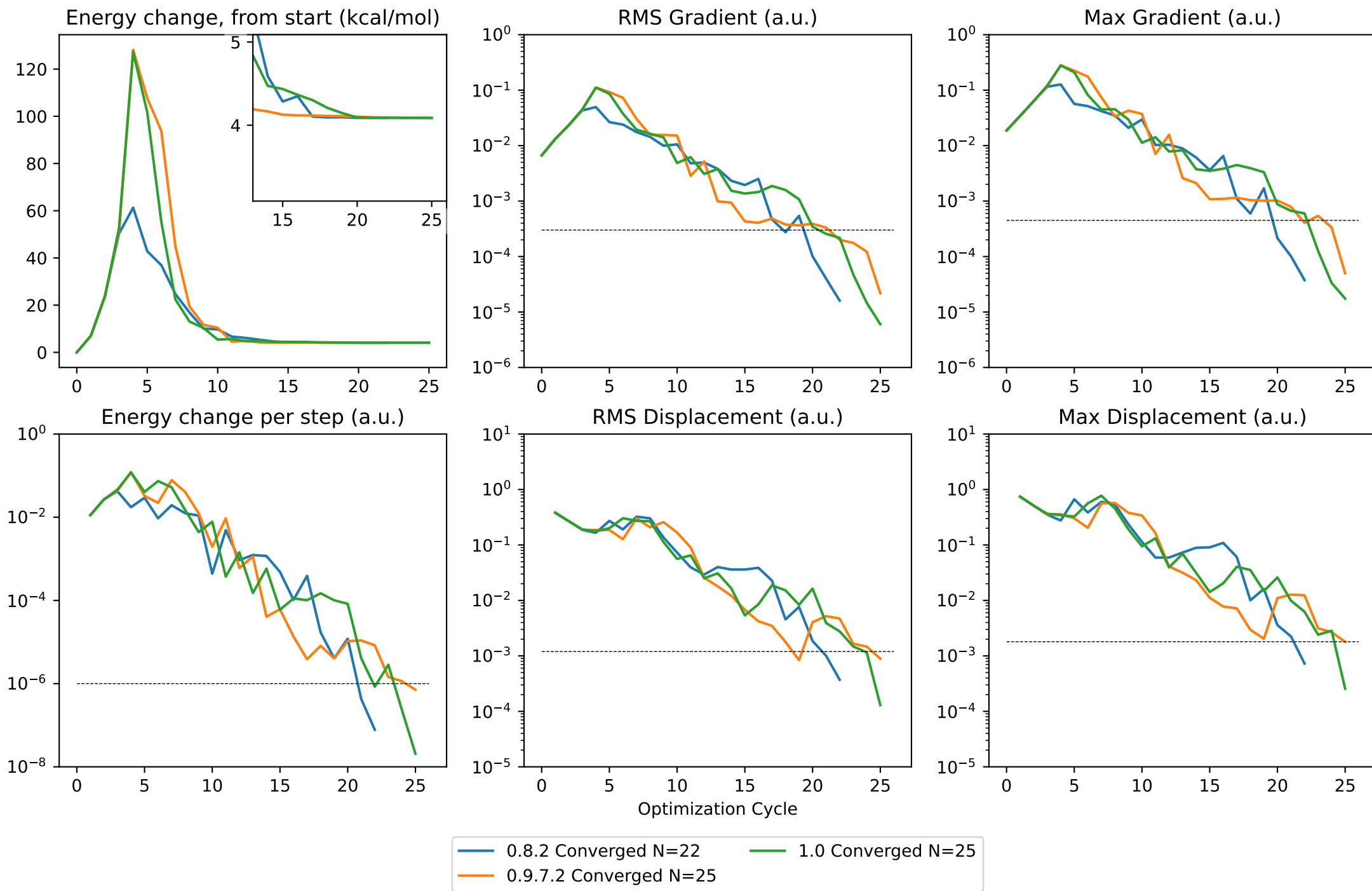


0.8.2 Converged N=59 1.0 Converged N=59
0.9.7.2 Converged N=59

Optimization performance for dcb-tweezer

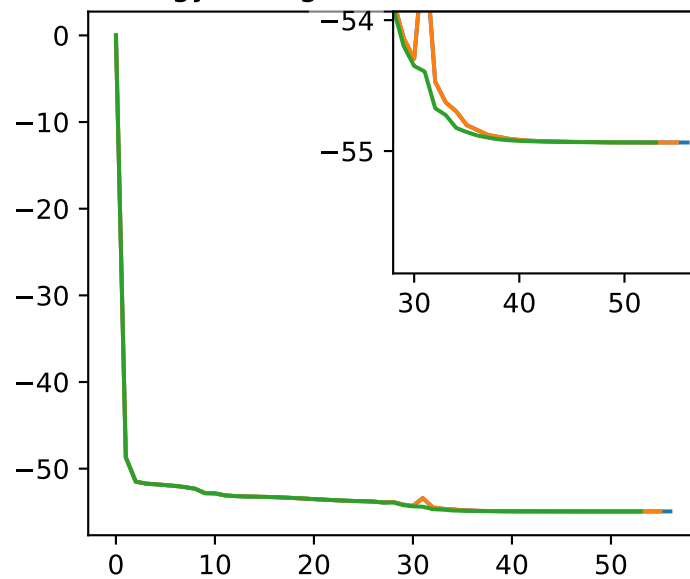


Optimization performance for diphenylmethane

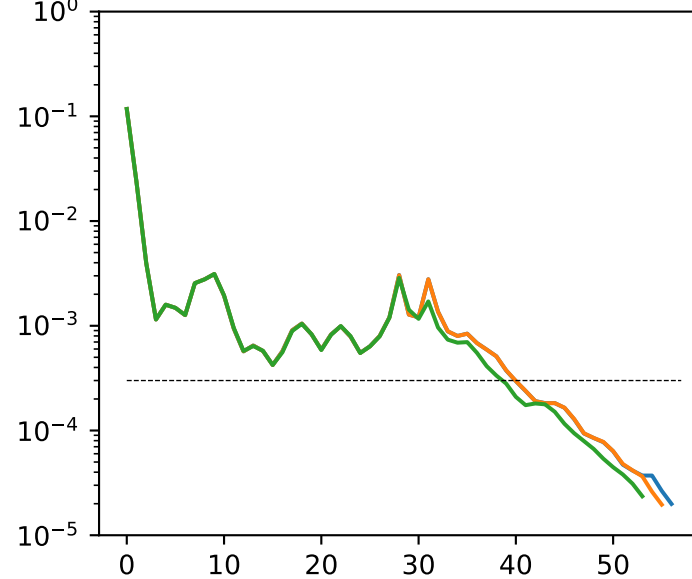


Optimization performance for fe4n_catalyst

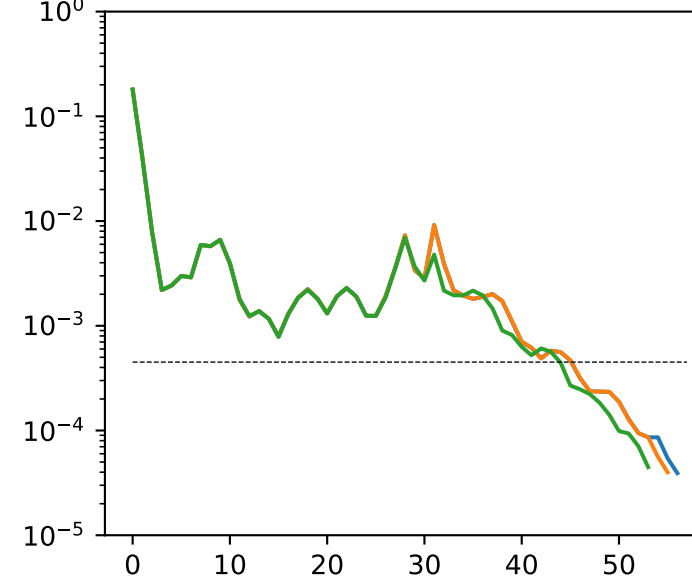
Energy change, from start (kcal/mol)



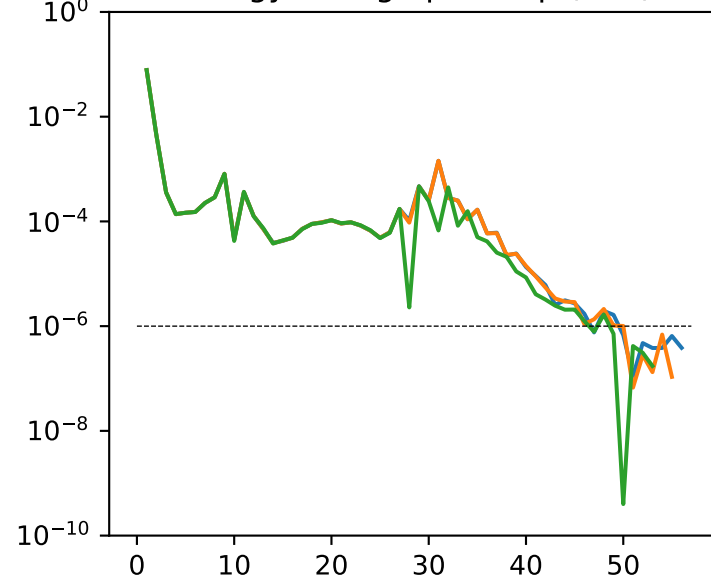
RMS Gradient (a.u.)



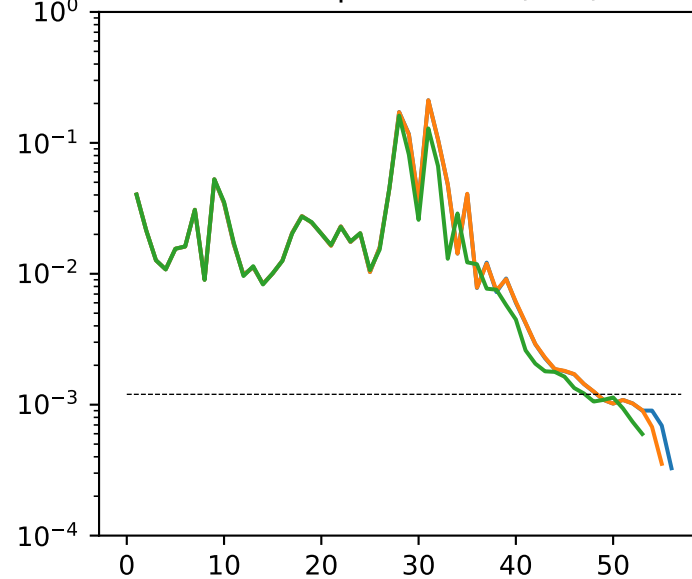
Max Gradient (a.u.)



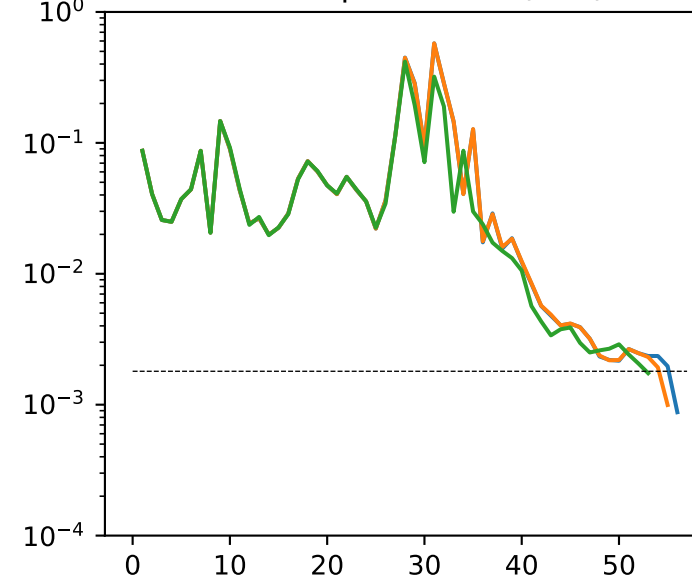
Energy change per step (a.u.)



RMS Displacement (a.u.)

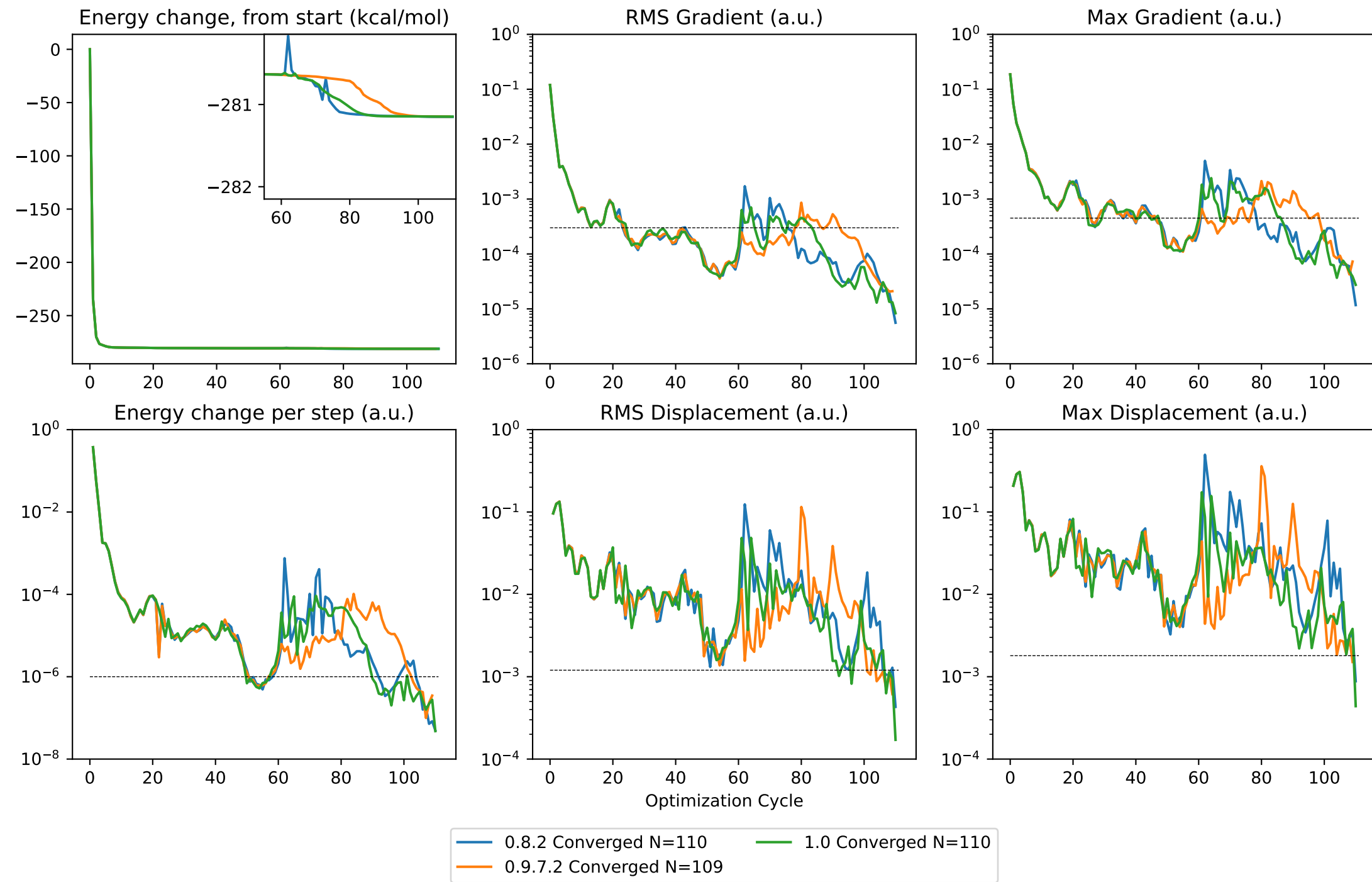


Max Displacement (a.u.)

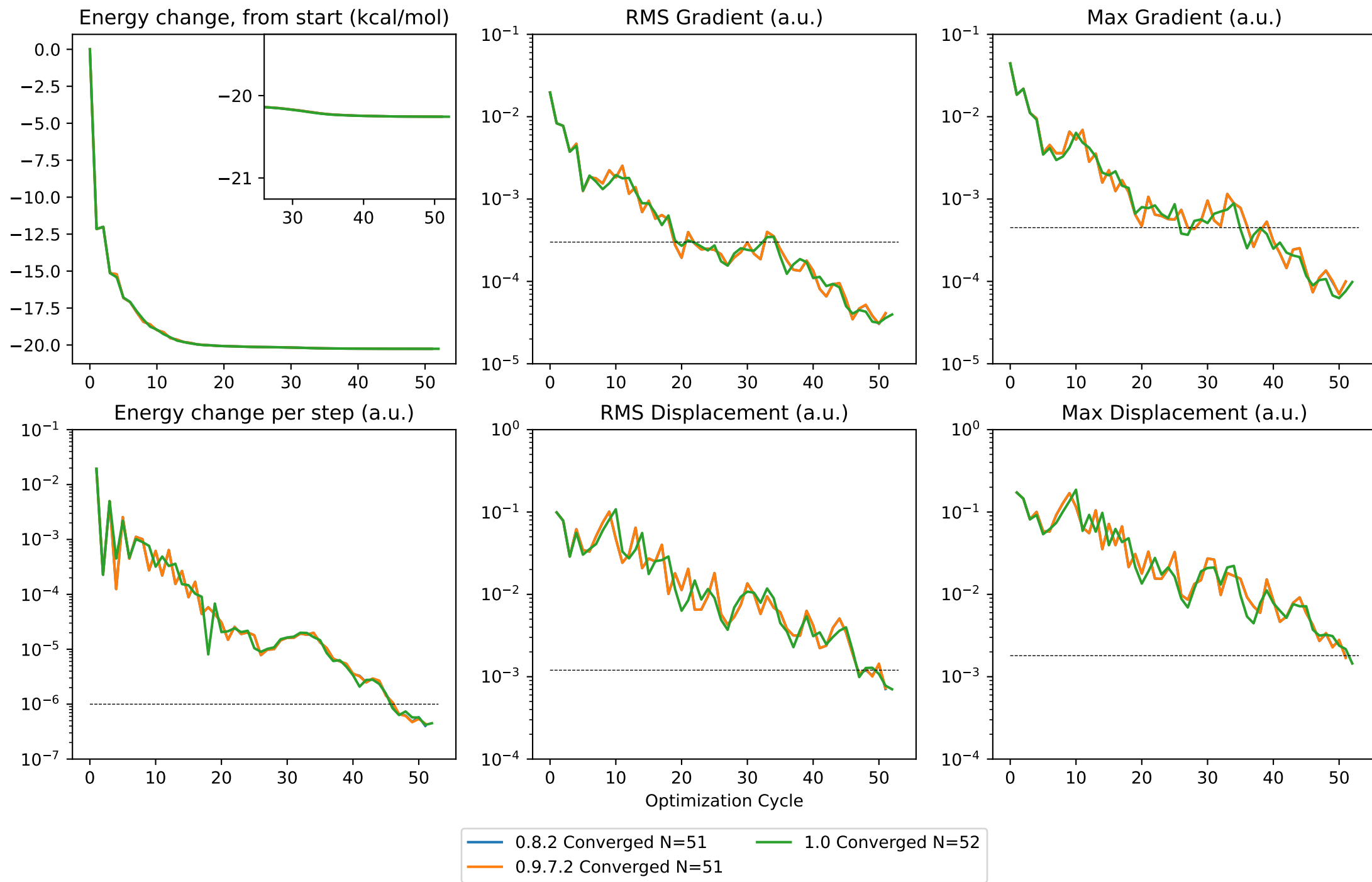


0.8.2 Converged N=56 1.0 Converged N=53
0.9.7.2 Converged N=55

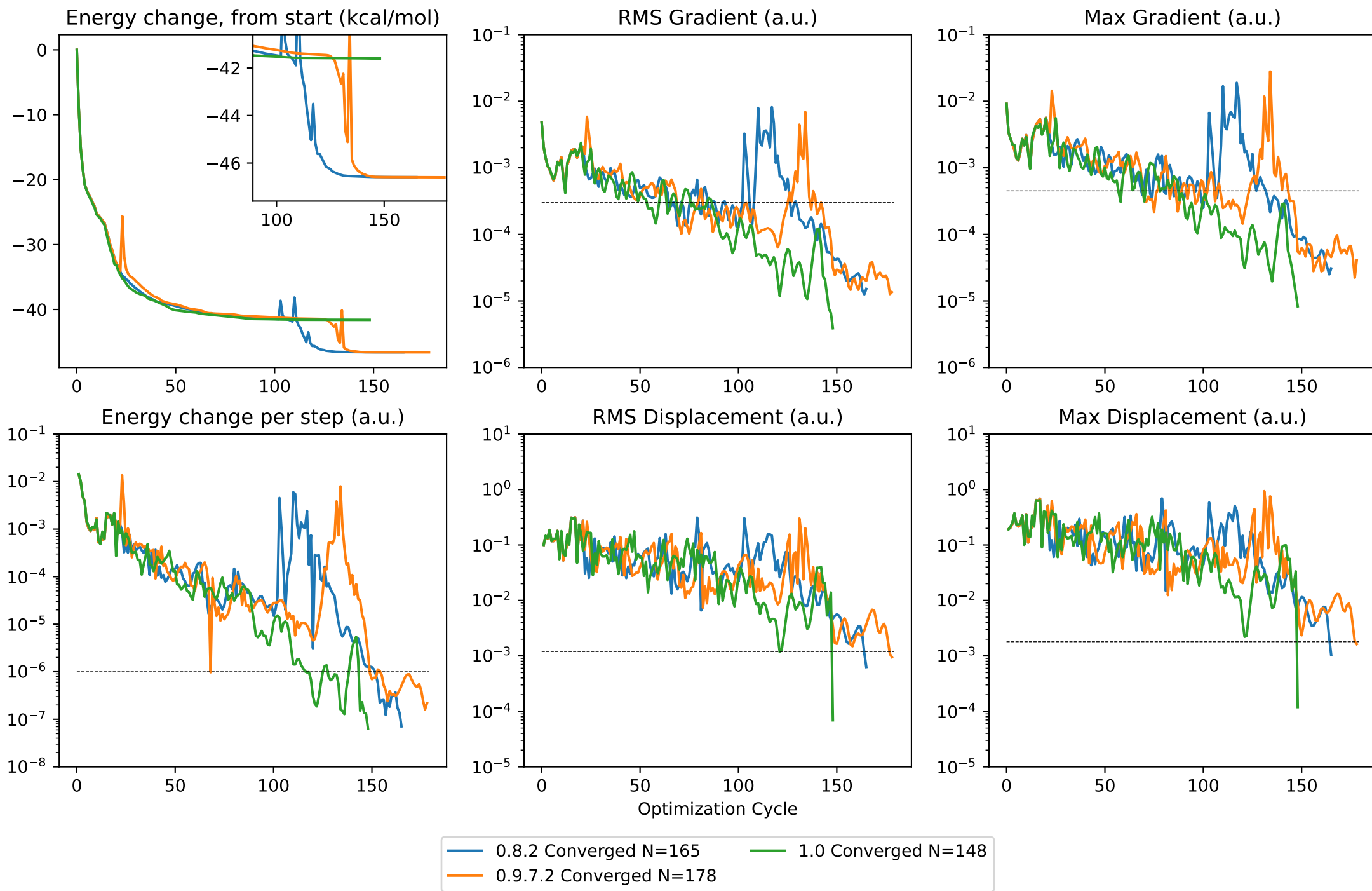
Optimization performance for fe-bpte-ncbh3



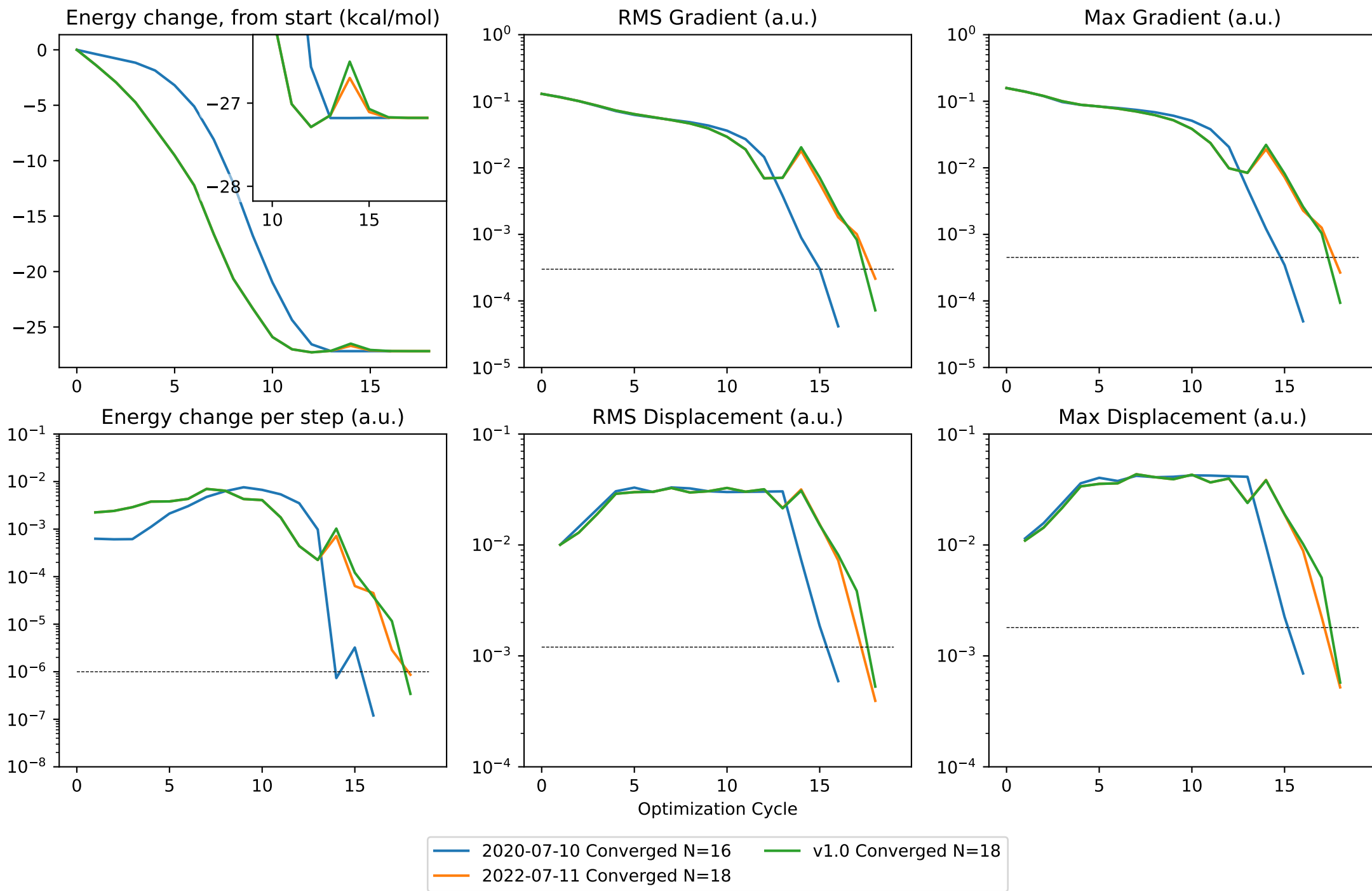
Optimization performance for gcgc-stack



Optimization performance for hccn_6

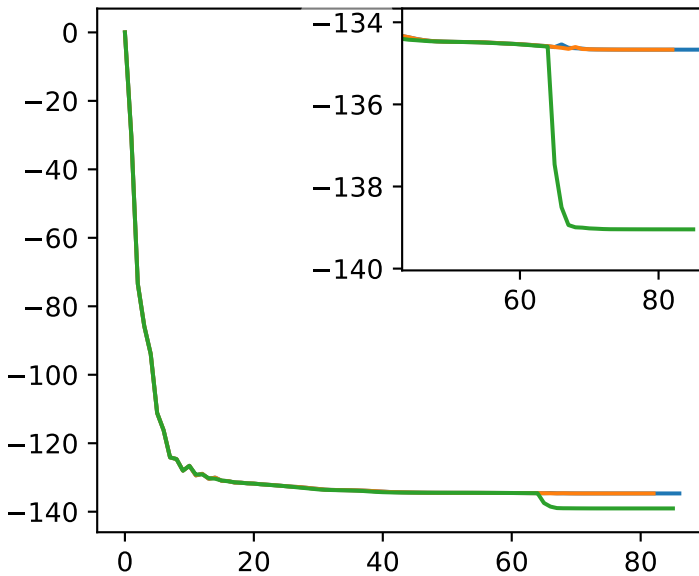


Optimization performance for hcn-hnc-ts

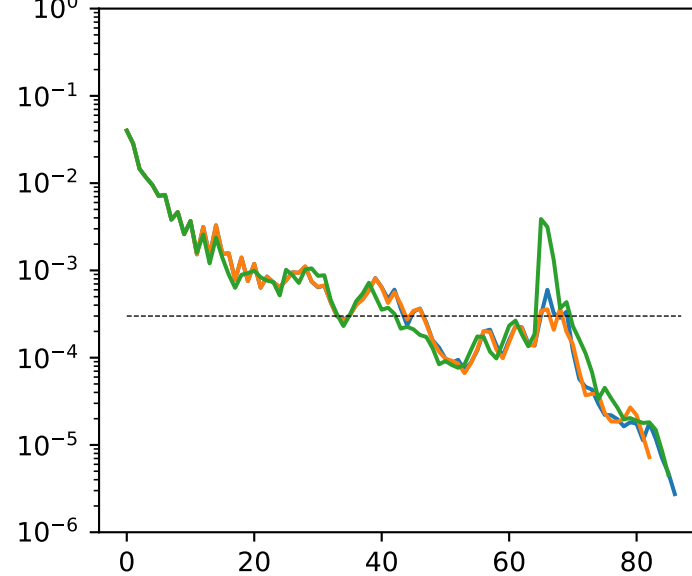


Optimization performance for heme

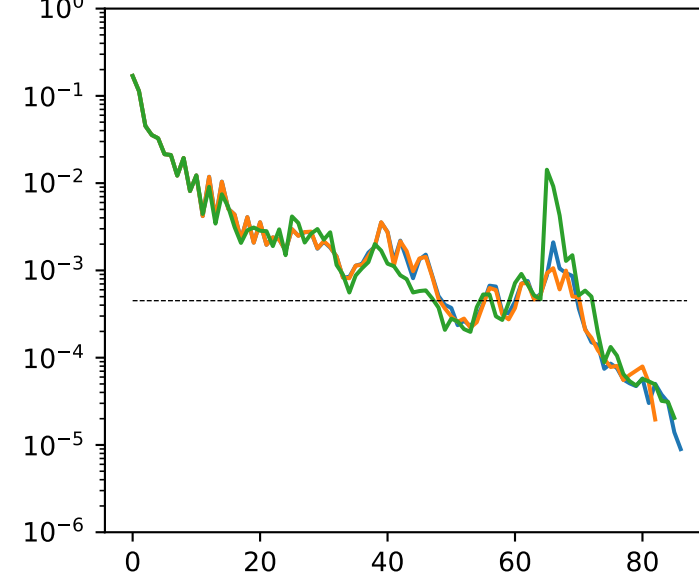
Energy change, from start (kcal/mol)



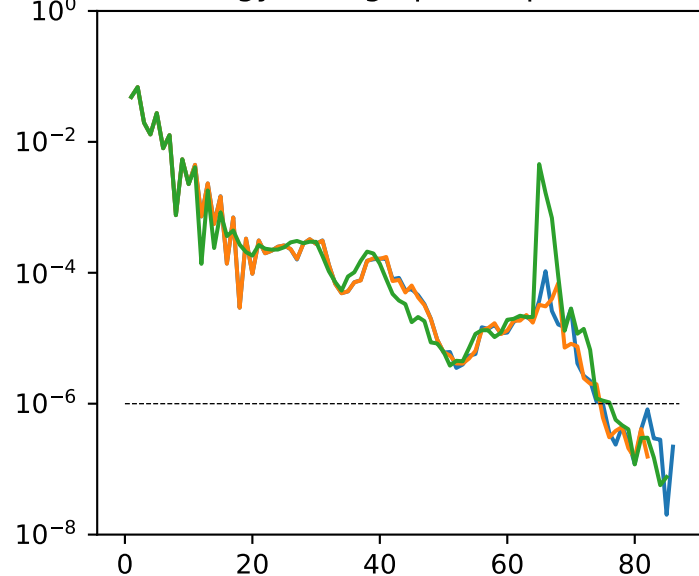
RMS Gradient (a.u.)



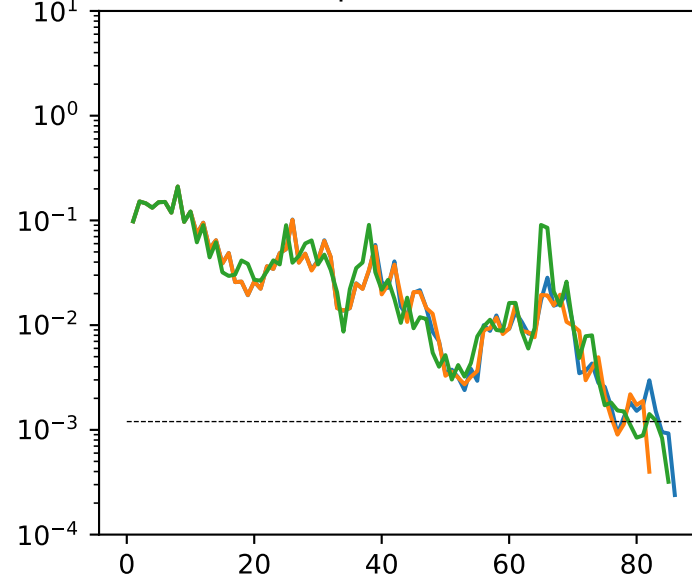
Max Gradient (a.u.)



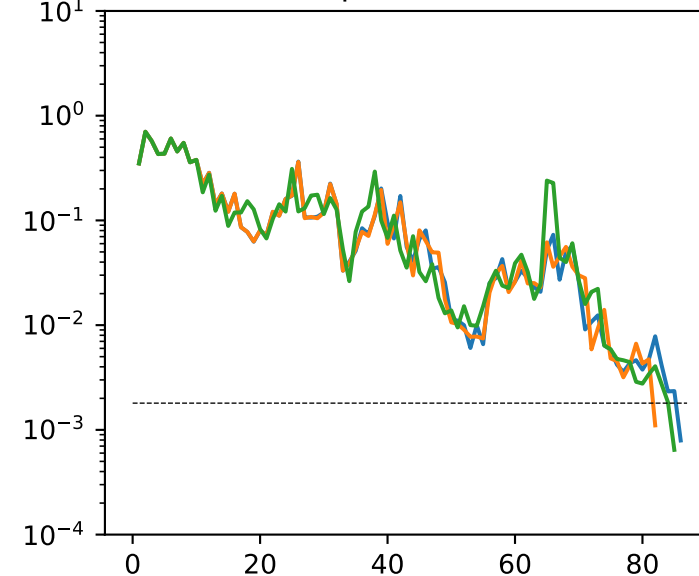
Energy change per step (a.u.)



RMS Displacement (a.u.)



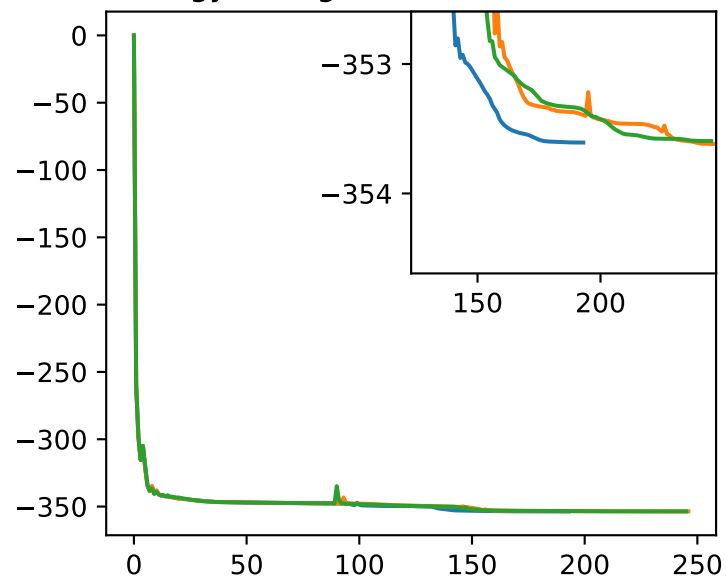
Max Displacement (a.u.)



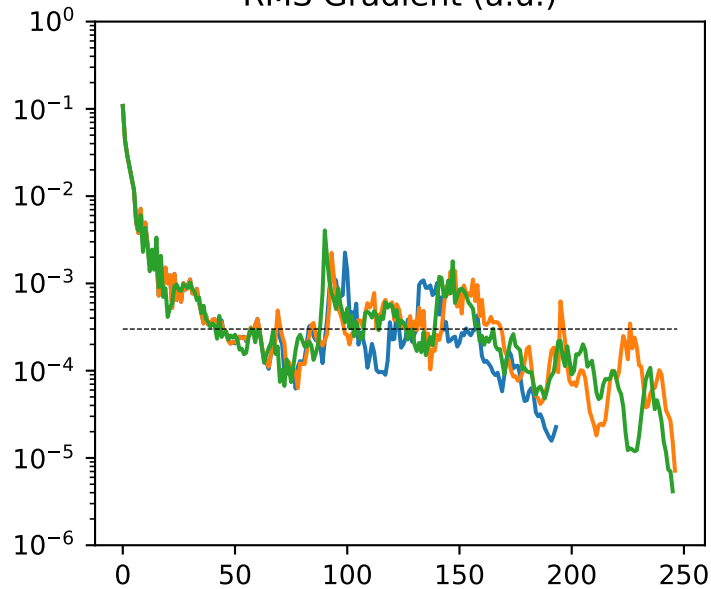
— 0.8.2 Converged N=86 — 1.0 Converged N=85
— 0.9.7.2 Converged N=82

Optimization performance for imatinib-salt

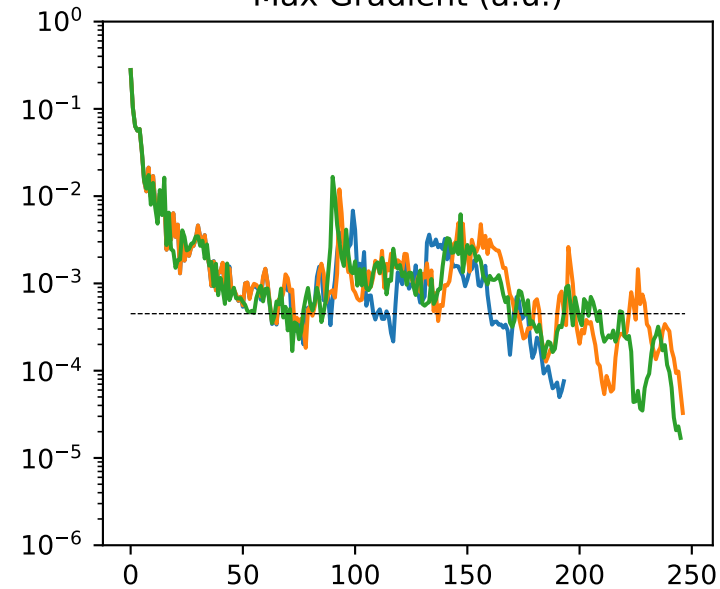
Energy change, from start (kcal/mol)



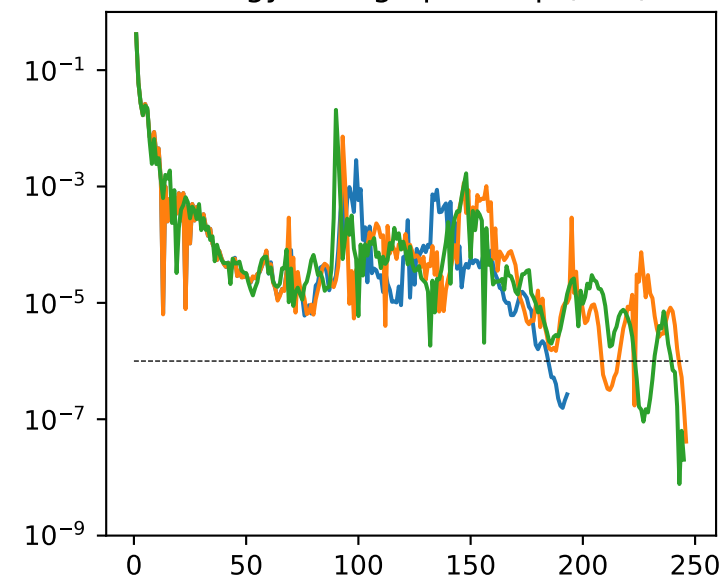
RMS Gradient (a.u.)



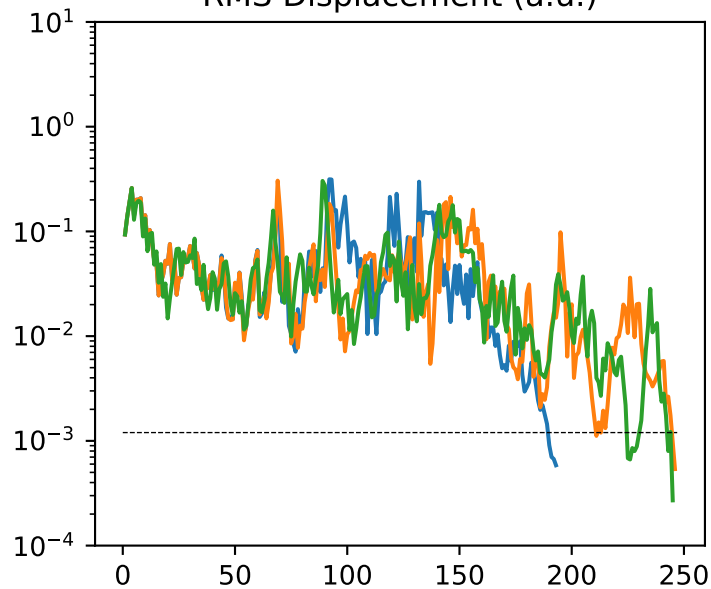
Max Gradient (a.u.)



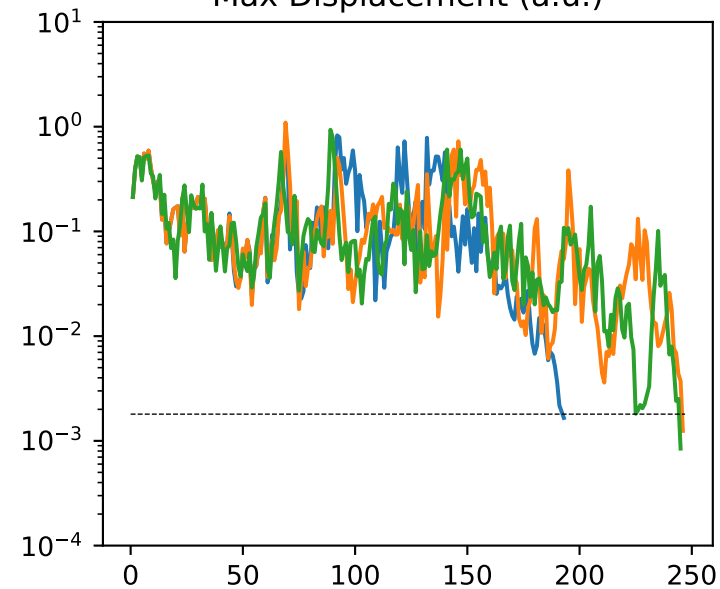
Energy change per step (a.u.)



RMS Displacement (a.u.)



Max Displacement (a.u.)

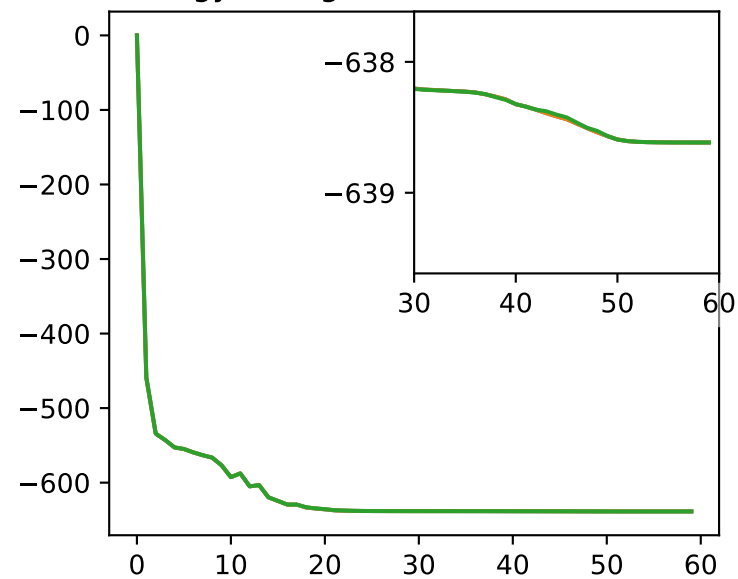


Optimization Cycle

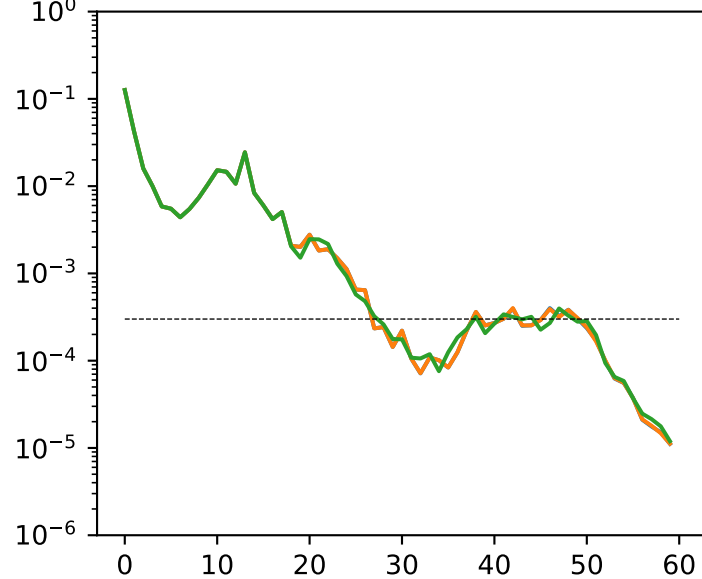


Optimization performance for ivermectin

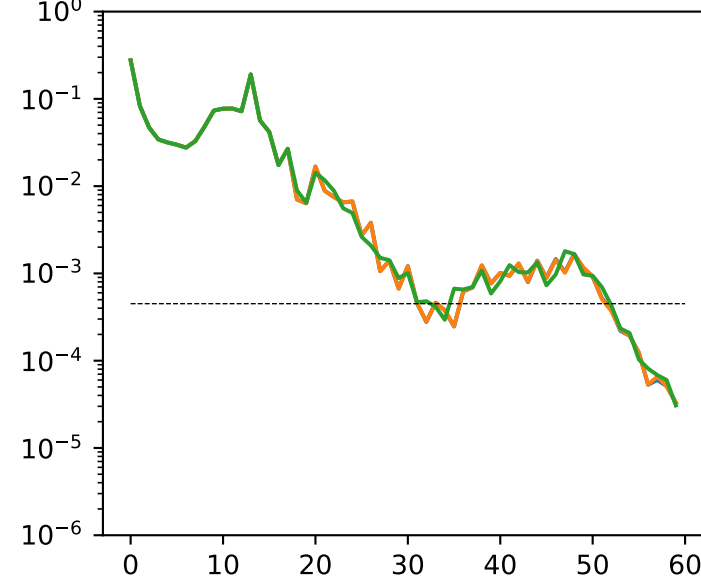
Energy change, from start (kcal/mol)



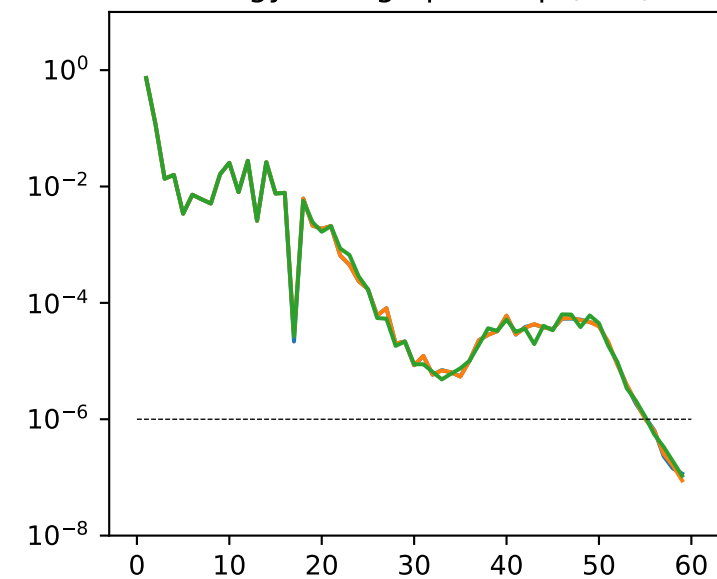
RMS Gradient (a.u.)



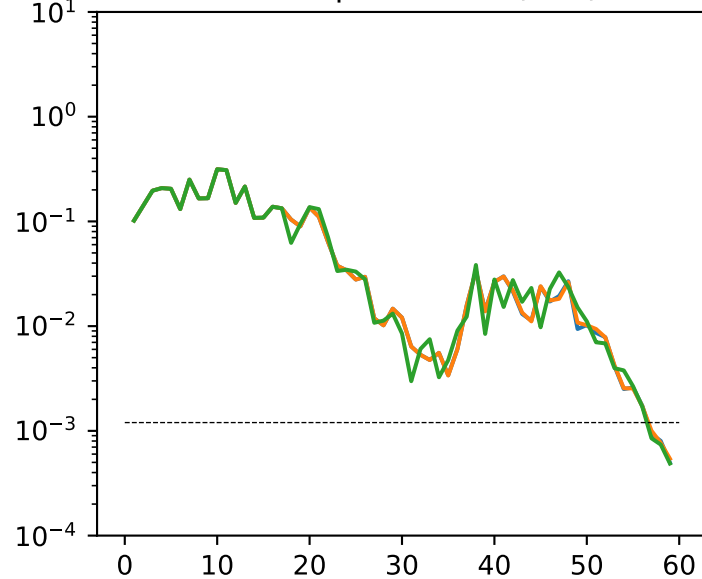
Max Gradient (a.u.)



Energy change per step (a.u.)



RMS Displacement (a.u.)

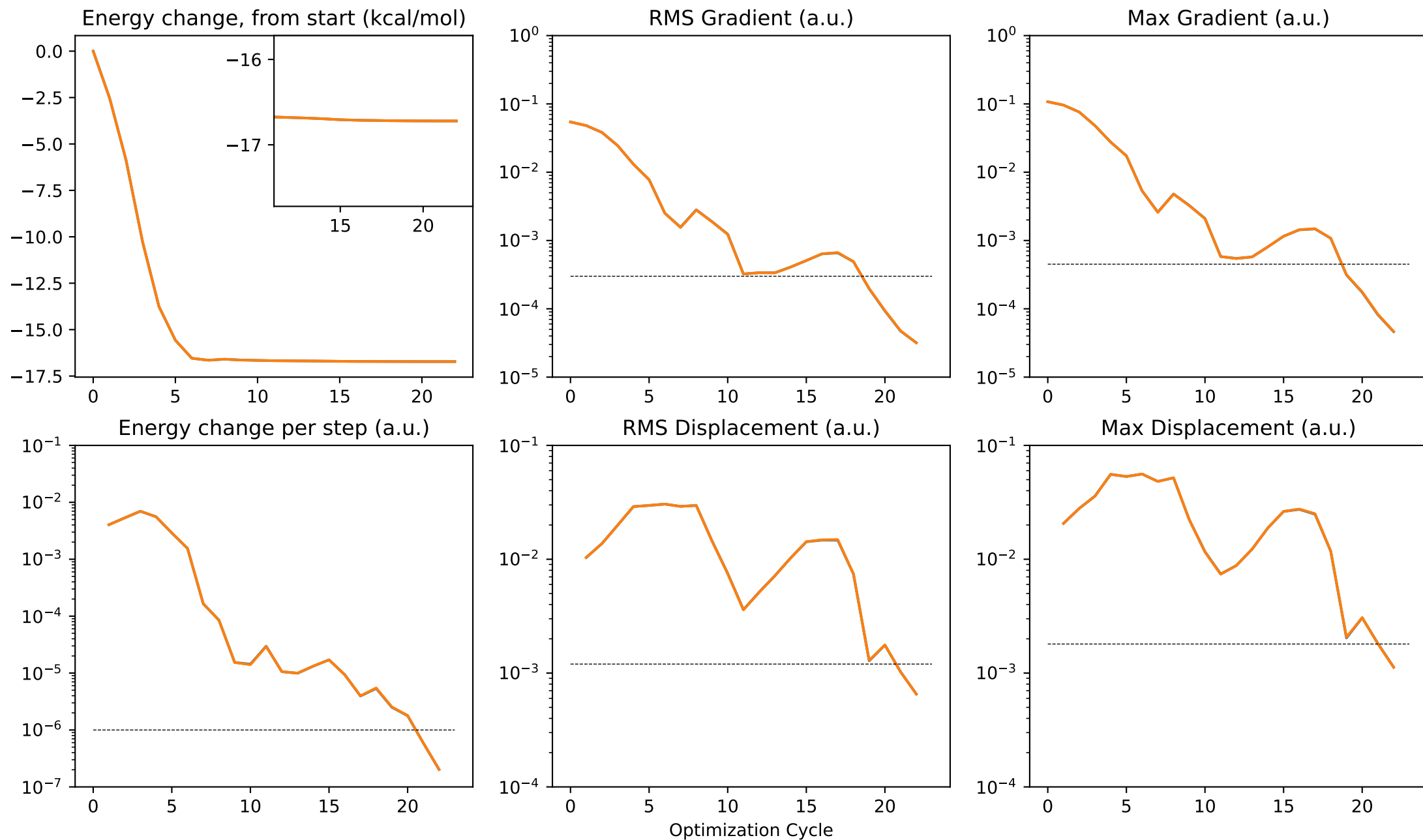


Max Displacement (a.u.)



— 0.8.2 Converged N=59 — 1.0 Converged N=59
— 0.9.7.2 Converged N=59

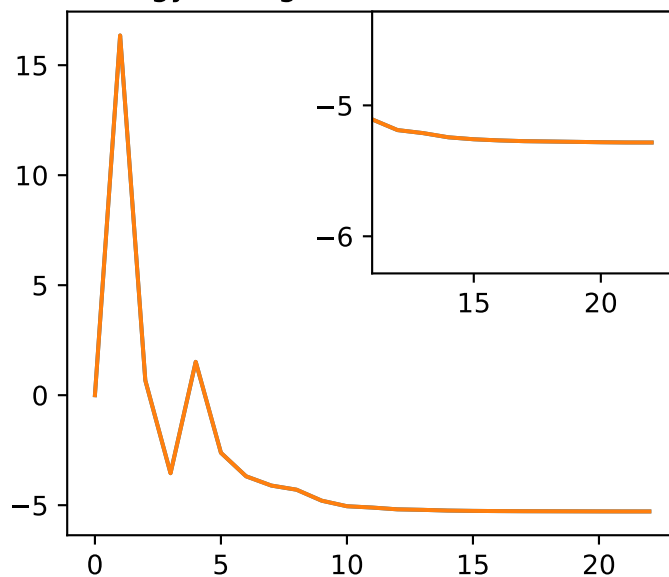
Optimization performance for malonate-ts



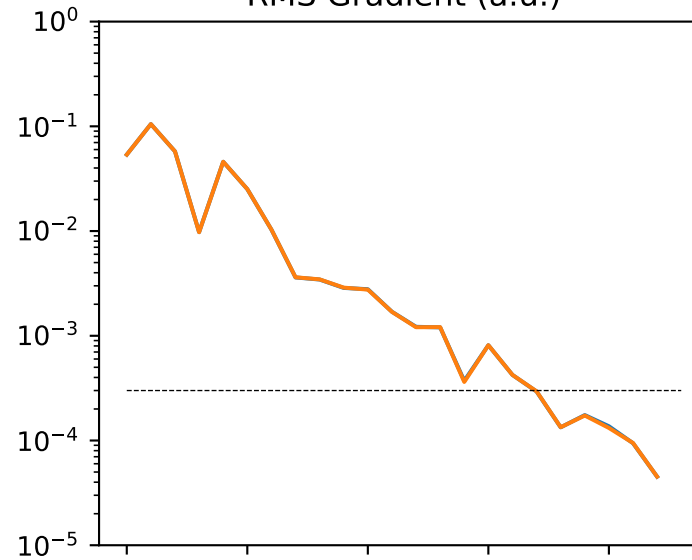
2022-08-12 Converged N=22 v1.0 Converged N=22

Optimization performance for psb3-qmmm-meci

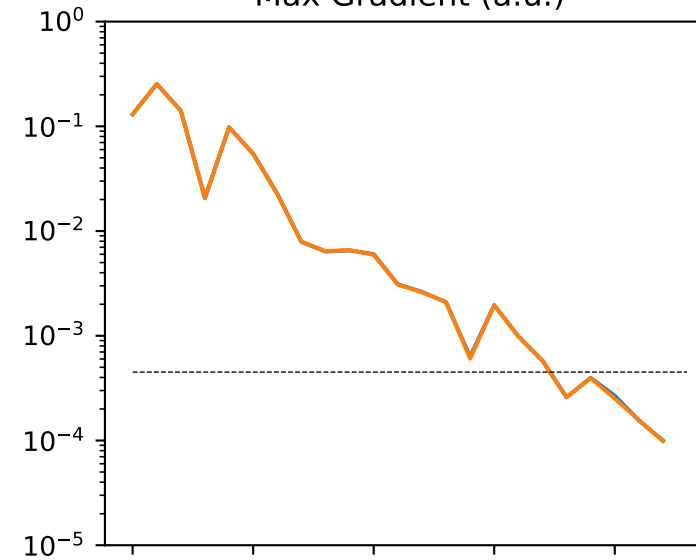
Energy change, from start (kcal/mol)



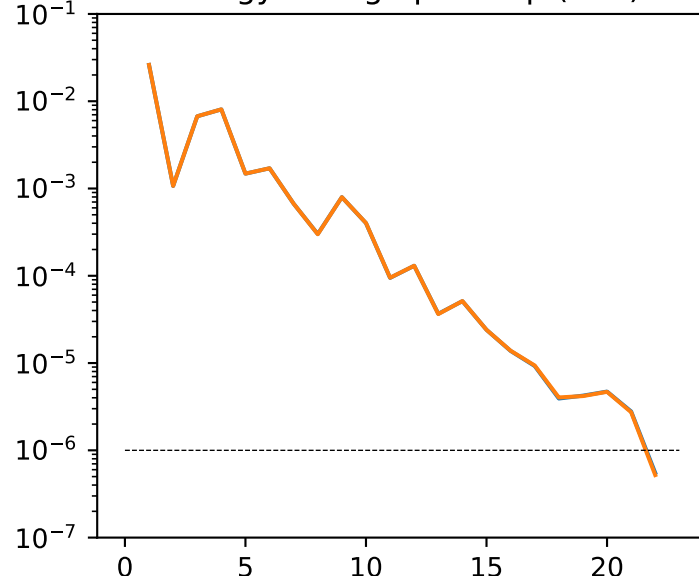
RMS Gradient (a.u.)



Max Gradient (a.u.)



Energy change per step (a.u.)



RMS Displacement (a.u.)



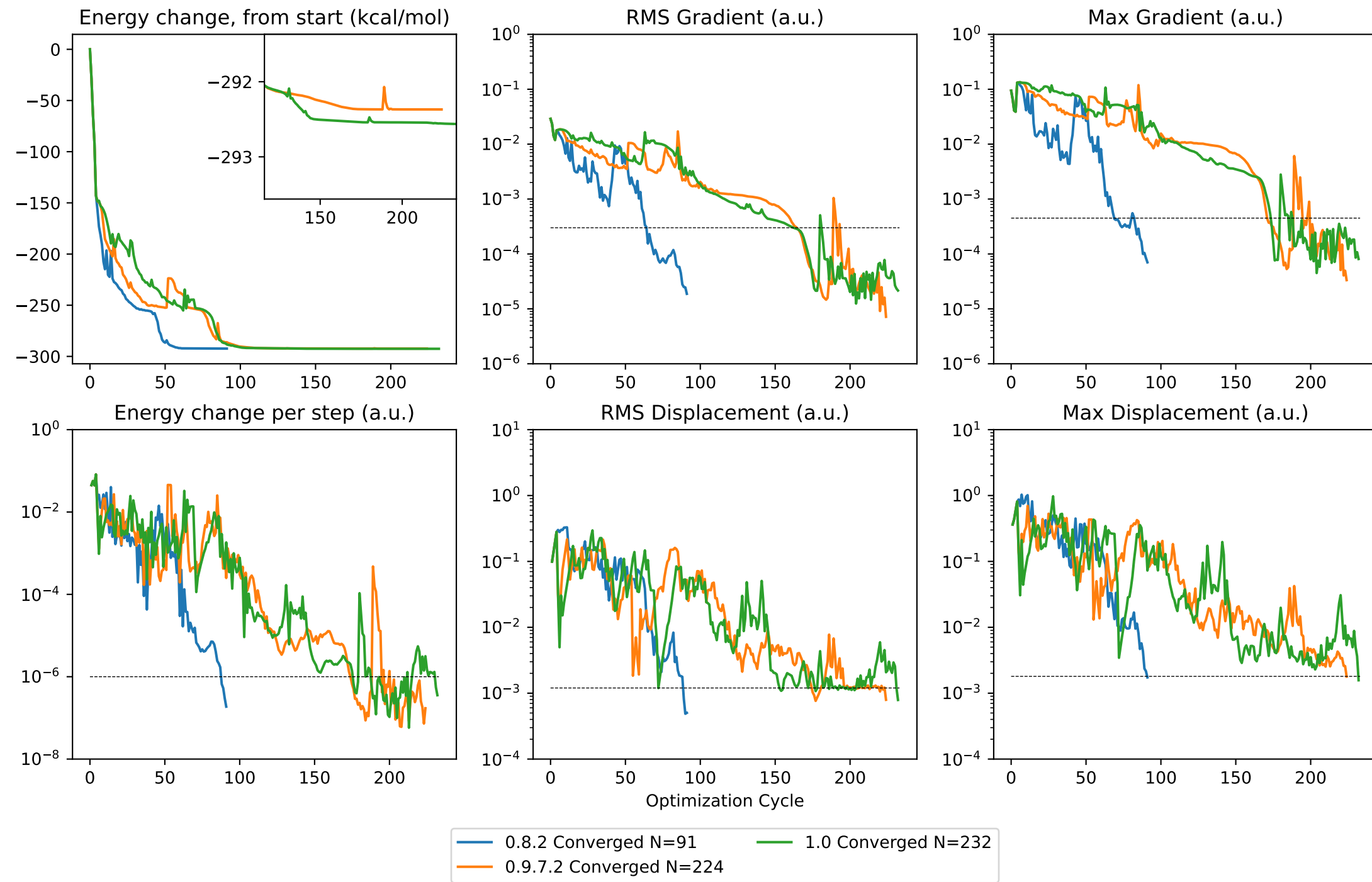
Max Displacement (a.u.)



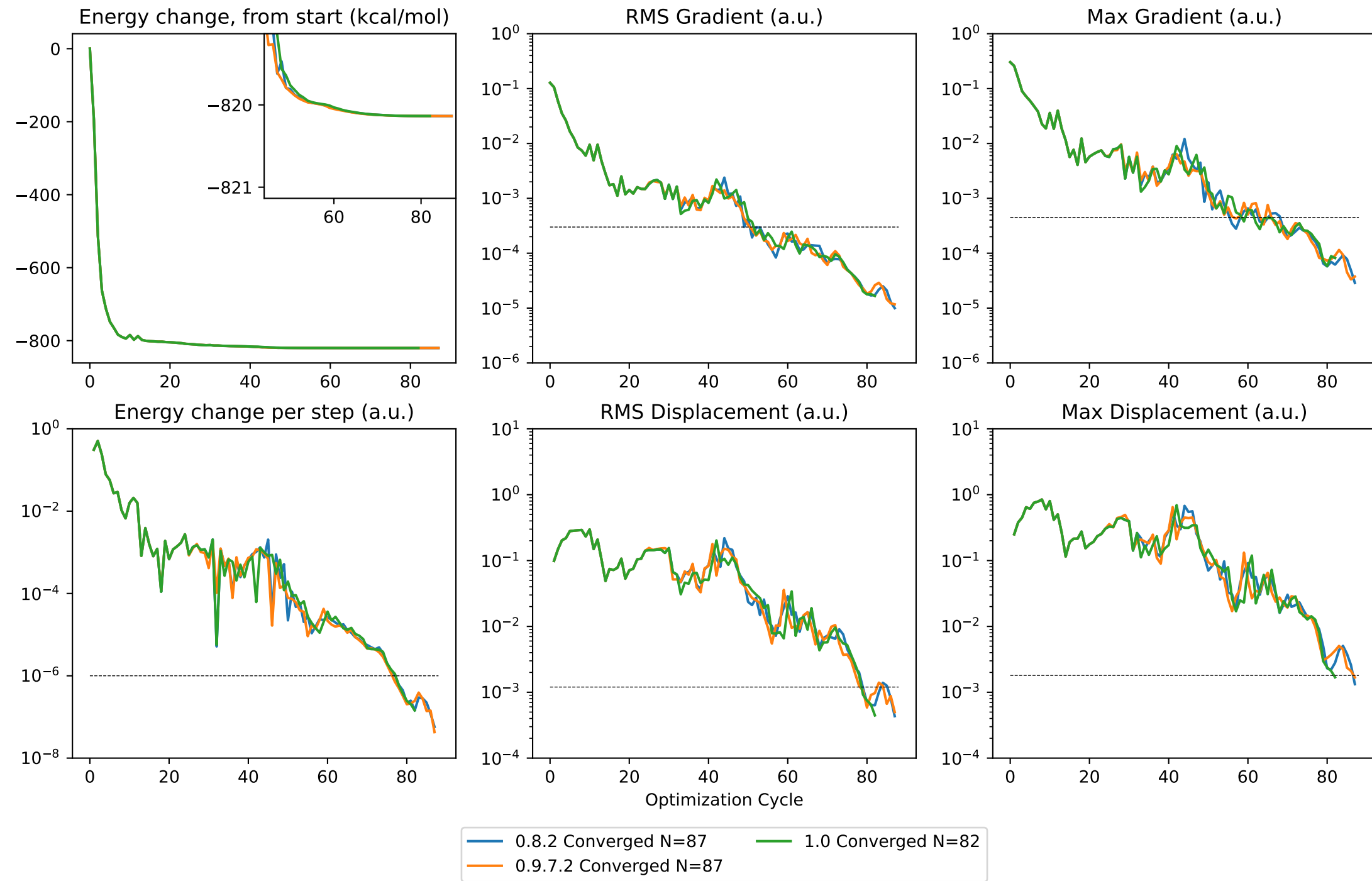
Optimization Cycle

2022-09-08 Converged N=22 v1.0 Converged N=22

Optimization performance for sialyl-lewis-x

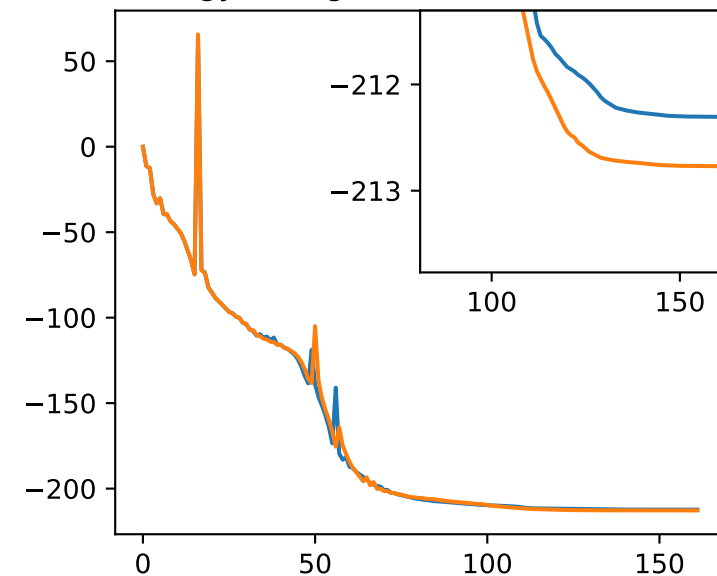


Optimization performance for taxol

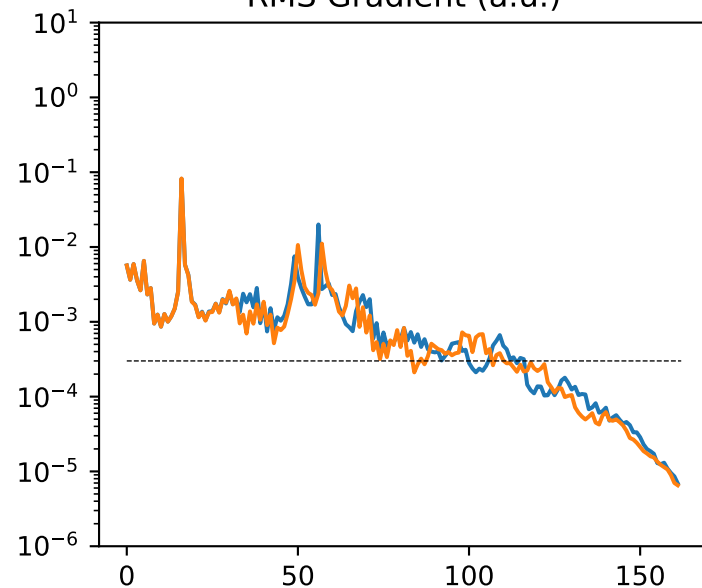


Optimization performance for trp-cage_openmm

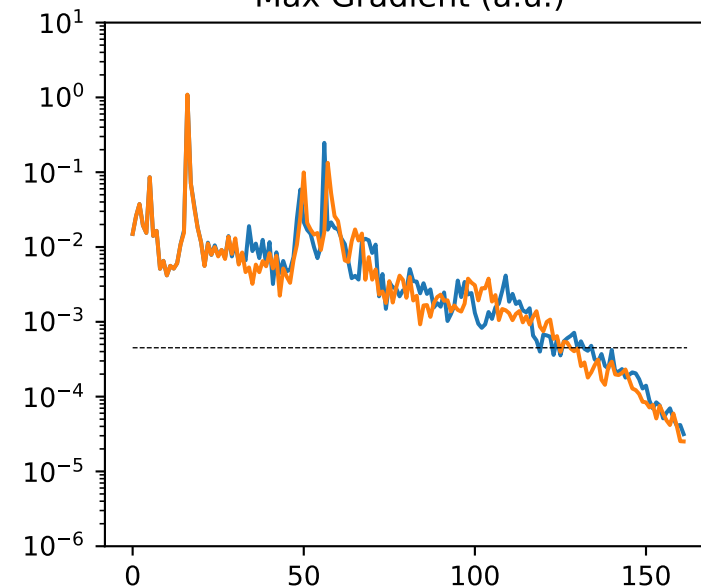
Energy change, from start (kcal/mol)



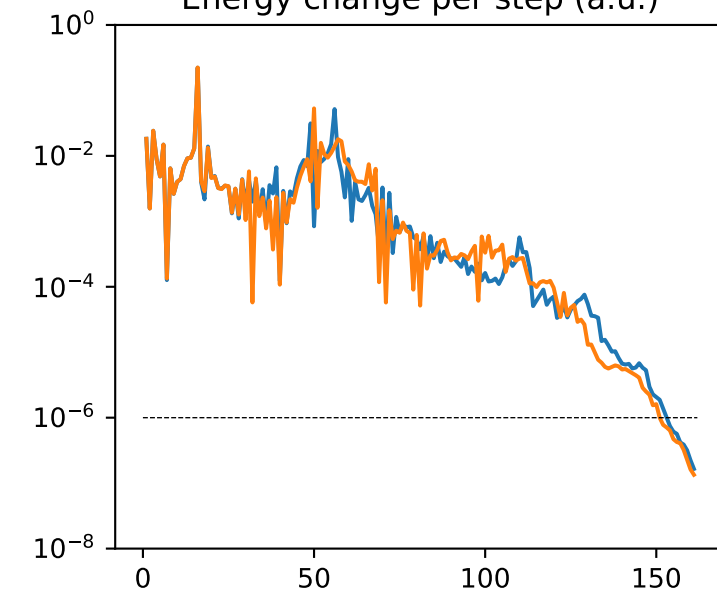
RMS Gradient (a.u.)



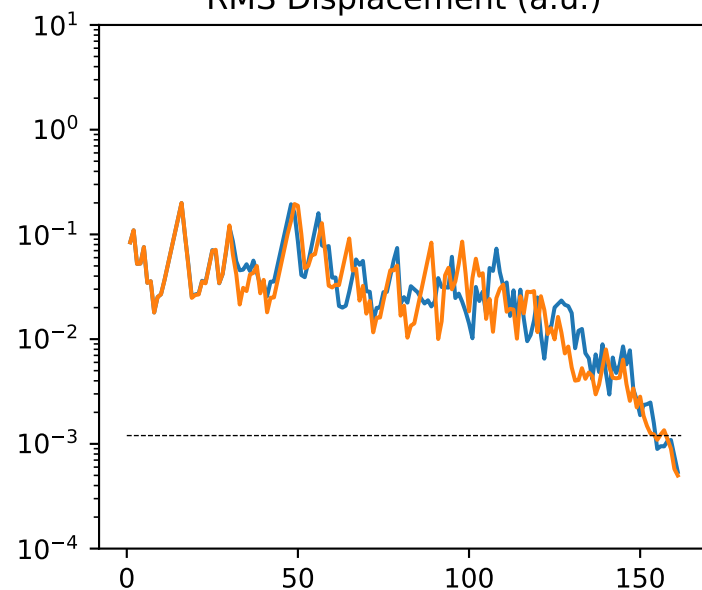
Max Gradient (a.u.)



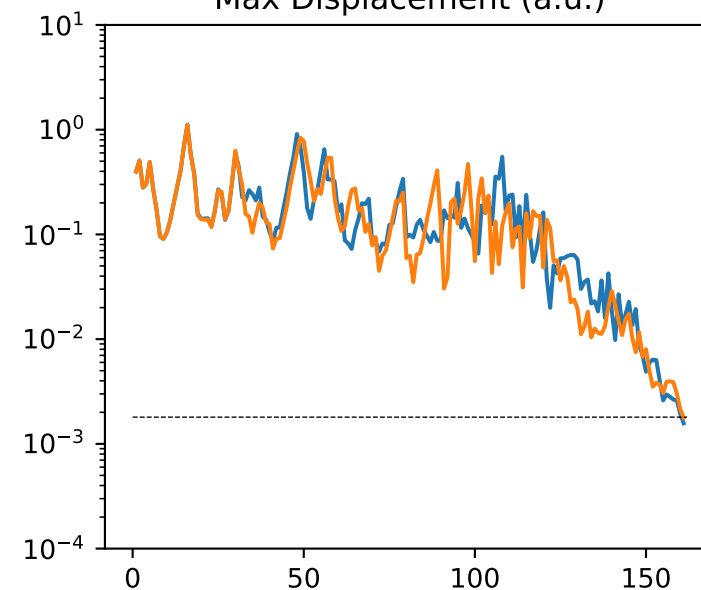
Energy change per step (a.u.)



RMS Displacement (a.u.)

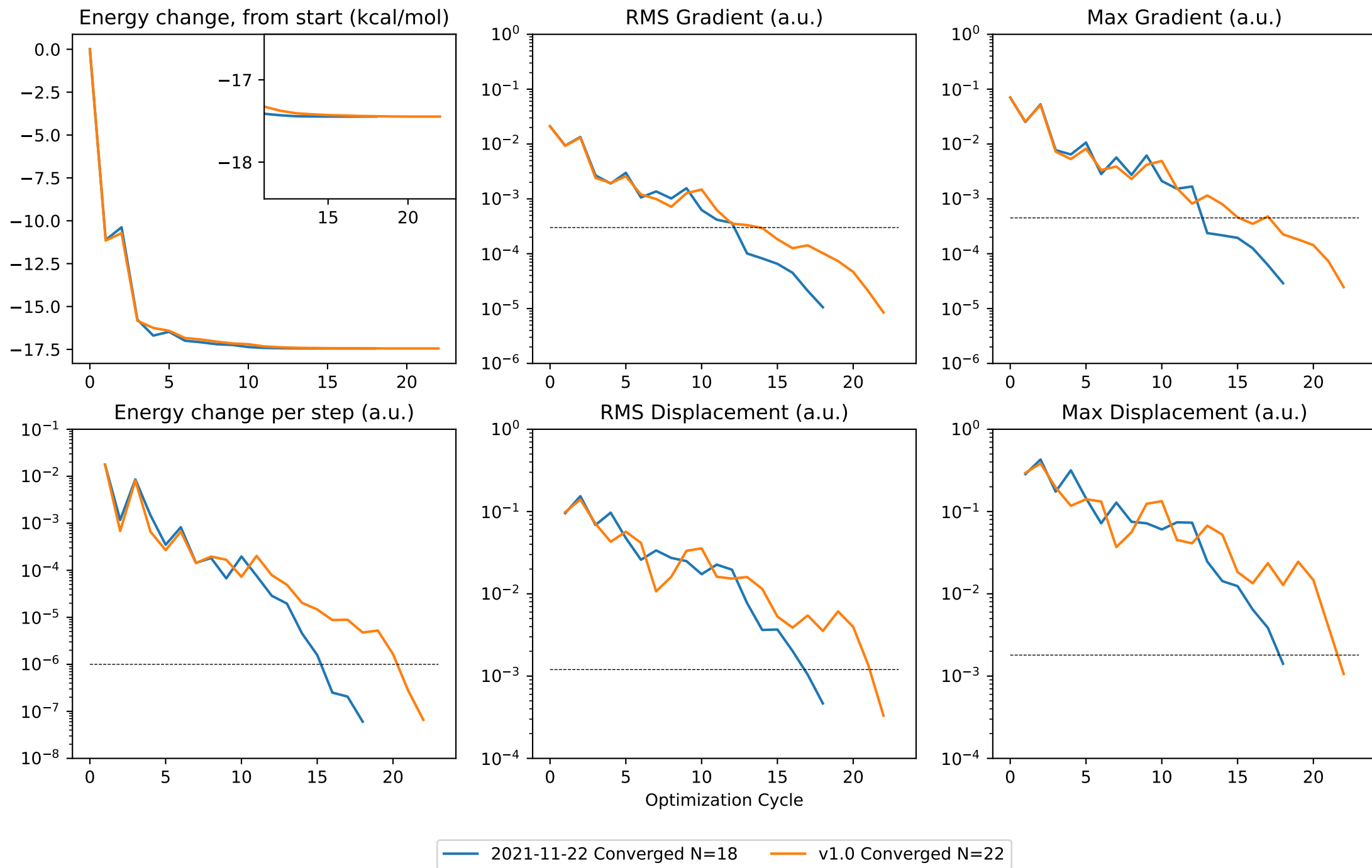


Max Displacement (a.u.)

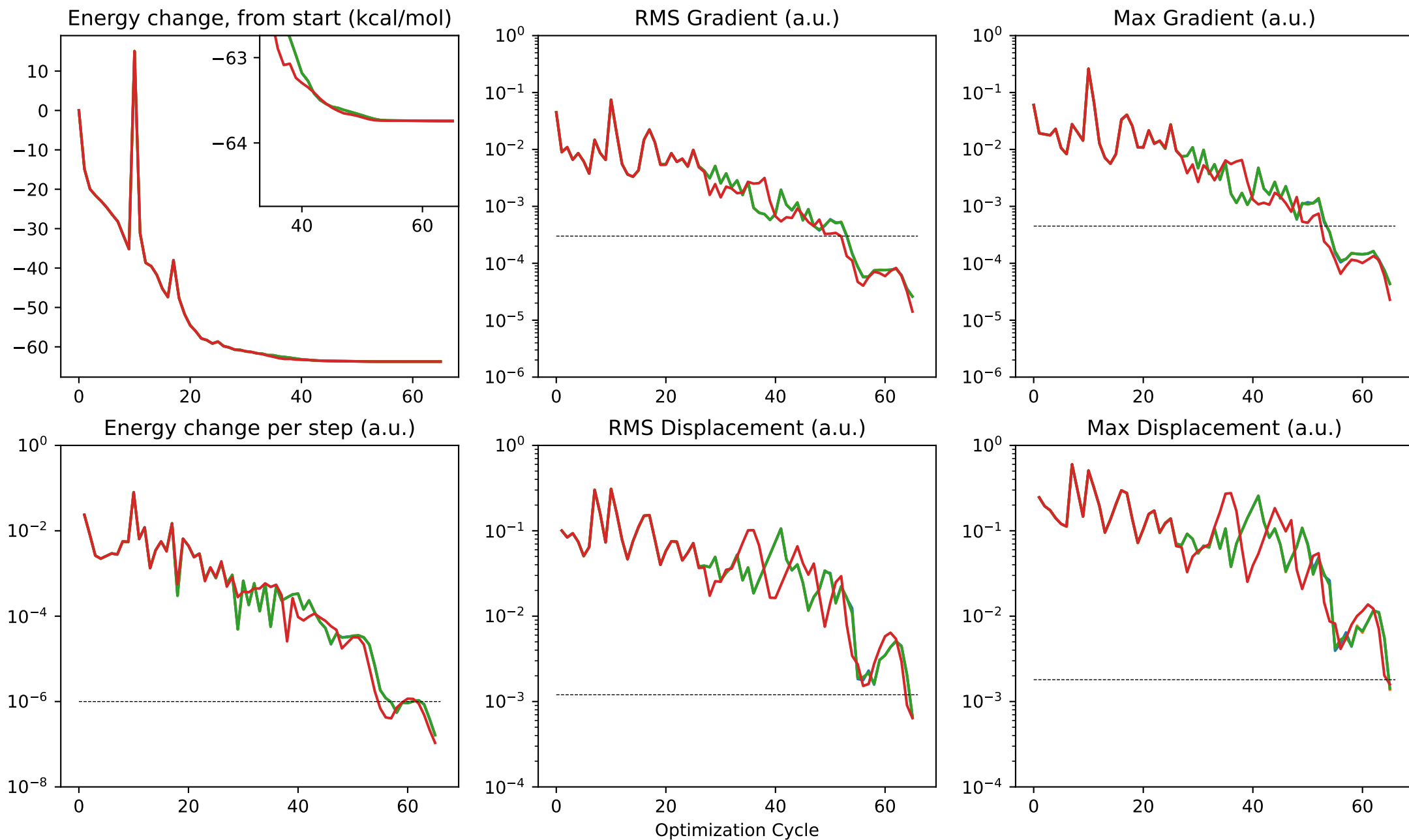


0.9.7.2 Converged N=161 1.0 Converged N=161

Optimization performance for vomilenine



Optimization performance for water6_qchem



2016-09-06 Converged N=65 v0.9.7.2 Converged N=65
 v0.8.2 Converged N=65 v1.0 Converged N=65