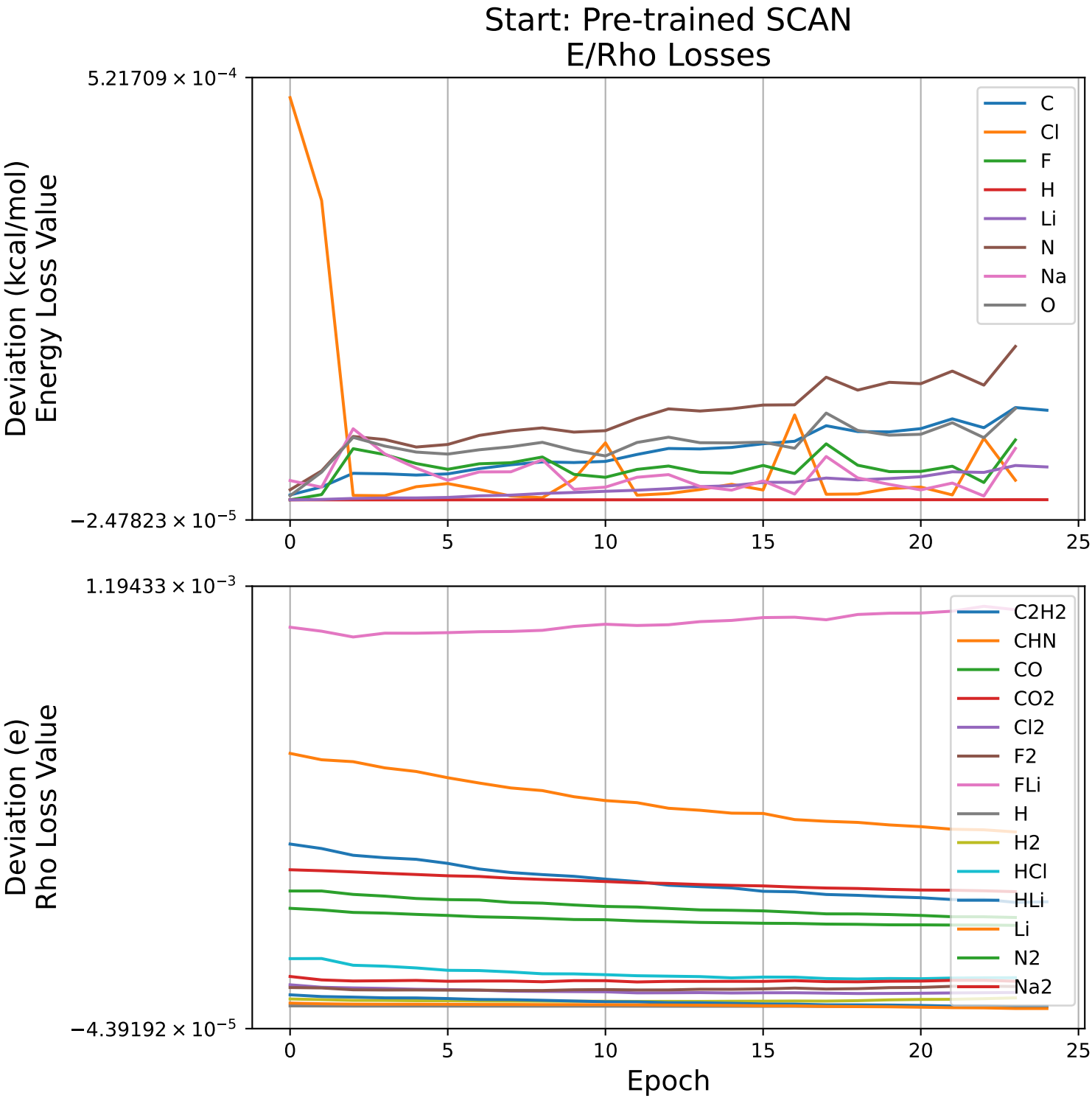
Start: Pre-trained SCAN
E/Rho Losses
Deviation (kcal/mol)
Energy Loss Value
5.21709×10^{-4}
-2.47823×10^{-5}
C
Cl
F
H
Li
N
Na
O
0
5
10
15
20
25
Deviation (e)
Rho Loss Value
1.19433×10^{-3}
-4.39192×10^{-5}
C2H2
CHN
CO
CO2
Cl2
F2
FLi
H
H2
HCl
HLi
Li
N2
Na2
Epoch