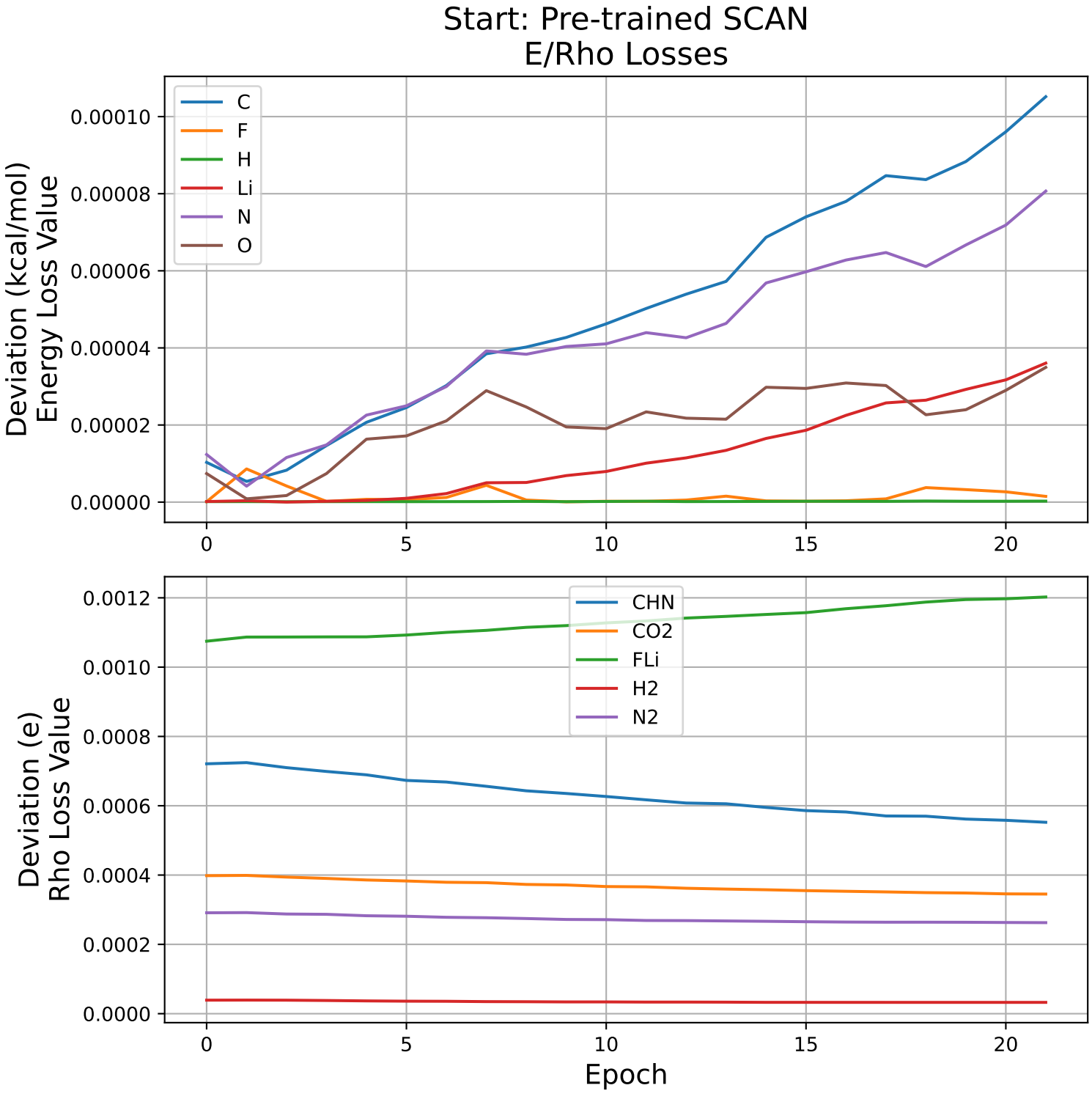
Start: Pre-trained SCAN
E/Rho Losses
Deviation (kcal/mol)
Energy Loss Value
C
F
H
Li
N
O
0.00010
0.00008
0.00006
0.00004
0.00002
0.00000
0
5
10
15
20
Deviation (e)
Rho Loss Value
CHN
CO2
FLi
H2
N2
0.0012
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
0
5
10
15
20
Epoch