Start: Pre-trained SCAN **Aggregate Losses** 10³ Ε ae rho Total 10² Deviation (kcal/mol) 10¹ 10⁰ 0 -10^{0} -10^{1} 2.5 5.0 10.0 12.5 15.0 17.5 20.0 0.0 7.5 **Epoch**