Start: Pre-trained SCAN **Aggregate Losses** 10⁴ 10³ 10^{2} Deviation (kcal/mol) 10^{1} 10⁰ 0 -10^{0} -10^{1} -10^{2} Е ae -10^{3} rho Total 200 50 100 150 250 300 350 400 **Epoch**