Start: Pre-trained SCAN **Aggregate Losses**  $10^{4}$ 10<sup>3</sup> 10<sup>2</sup> Deviation (kcal/mol)  $10^{1}$ 10<sup>0</sup> 0 -10°  $-10^{1}$  $-10^{2}$ Ε ae  $-10^{3}$ rho Total 50 100 150 200 250 300 350 400 **Epoch**