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