Start: Pre-trained SCAN **Aggregate Losses** Ε ae rho Total 10<sup>3</sup>  $10^{2}$ Deviation (kcal/mol)  $10^1$ 10<sup>0</sup> 0  $-10^{0}$  $-10^{1}$  $-10^{2}$ 5 . 25 10 15 20 **Epoch**