A graph of different colored lines

AI-generated content may be incorrect.

As expected, the computed diffusion coefficient decreases as chain length increases since longer polymer chains diffuse more slowly due to increased entanglement and drag. That pattern confirms that the MD code is capturing the overall physics of polymer diffusion.

I also tested different RescaleFreq values, which led to different D values. This makes sense since RescaleFreq determines how velocity is rescaled to maintain the target temperature T. At RescaleFreq = 100, the velocities are rescaled frequently, and the system is continuously adjusted to maintain the target temperature. However, this may prevent the system from naturally exploring its phase space. A higher RescaleFreq should allow the polymer chain to diffuse more naturally. But in the case RescaleFreq=100 trends downward as M increases.

A confusing result appears around M = 8 and M = 12, where there is an increase in D for some rescaling frequencies. This could be due to statistical noise from finite sampling. Given additional time, I would increase the number of production steps to see if the trend stabilizes, regardless of RescaleFreq. I would also run MD simulations multiple times per M to ensure reliable averages. Additionally, I would examine the trajectories for M > 8 to check for any explanation for the increase in D.