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N-terminal prion protein peptides (PrP(120–144)) form parallel in-register β-sheets via multiple nucleation-dependent pathways.

Yiming Wang, Qing Shao, and Carol K. Hall

In the "Materials and Methods" section, the conversion of the reduced time unit to a real time unit ($\Delta t^* = 0.072$ ns) was incorrect. The correct value should be $\Delta t^* = 0.96$ ns. Thus, the longest time accessed in the single DMD simulation should have been 672 μs, which corresponds to 2000 billion collisions. The simulation times (x axes) in Figs. 1, 6, 7, and 9 and Figs. S1–S5 and Table 2 as well as in other places in the context of the article should all be multiplied by a factor of 29. The correct calculation procedures are described below.

The way that we relate the reduced time unit to the real time unit is to compare the self-diffusion coefficient of Aβ(16–22) peptide obtained from DMD simulation (D_{DMD}) and atomistic molecular dynamics (MD) simulation (D_{MD}) at $T = 298$ K. The reduced temperature of the self-diffusion coefficient measurement in DMD simulation is chosen to be $T^* = 0.181$, which corresponds to room temperature ($T = 298$ K) according to temperature scaling (Wang, Y., Shao, Q., and Hall, C. K. (2016) N-terminal prion protein peptides (PrP(120–144)) form parallel in-register β-sheets via multiple nucleation-dependent pathways. *J. Biol. Chem.* **291,** 22093–22105), $T^* = (T + 115.79)/2288.46 = (298 + 115.79)/2288.46 = 0.181$.

The self-diffusion coefficients in both DMD and MD simulation are calculated using the Einstein equation. We plotted the mean square displacement (MSD) of N Aβ(16–22) peptides *versus* time for both atomistic MD simulation ($N = 1$) and DMD simulation ($N = 6$), as shown in Fig. 11, *A* and *B*, by using the following equation,

$$\mathrm{MSD}(t + \Delta t) = \mathrm{MSD}(t) + \overline{d^2} = \mathrm{MSD}(t) + \frac{\sum_{i=1}^{i=N} |r_i^{t+\Delta t} - r_i^t|^2}{N} \quad \text{(Eq. 1)}$$

where Δt is the time unit; N is the total number of peptides; $\overline{d^2}$ is the averaged square displacement of N peptides; and $r_i^{t+\Delta t}$ and r_i^t are the coordinates of the ith peptide at $t + \Delta t$ and t. For DMD simulation, t^* is used in DMD instead of t to represent reduced time.

Using the MSD data in Fig. 11, *A* and *B*, we obtain the self-diffusion coefficients D_{MD} and D_{DMD}.

$$D_{MD} = \frac{1}{6}\frac{\mathrm{MSD}(t_2) - \mathrm{MSD}(t_1)}{t_2 - t_1} = \frac{48.11 - 27.45}{6 \times (17.80 - 10.66)} = 0.48\ \mathrm{nm^2/ns} \quad \text{(Eq. 2)}$$

$$D_{DMD} = \frac{1}{6}\frac{\mathrm{MSD}(t_2^*) - \mathrm{MSD}(t_1^*)}{t_2^* - t_1^*} = \frac{328.57 - 109.01}{6 \times (120.01 - 40.01)} = 0.46\ \mathrm{nm^2/\Delta t^*} \quad \text{(Eq. 3)}$$

By equating the self-diffusion coefficients calculated from both atomistic MD simulation and DMD simulation, we obtain the reduced time unit in DMD simulation in terms of the real time unit to be 1 (Δt^*) = 0.96 ns.

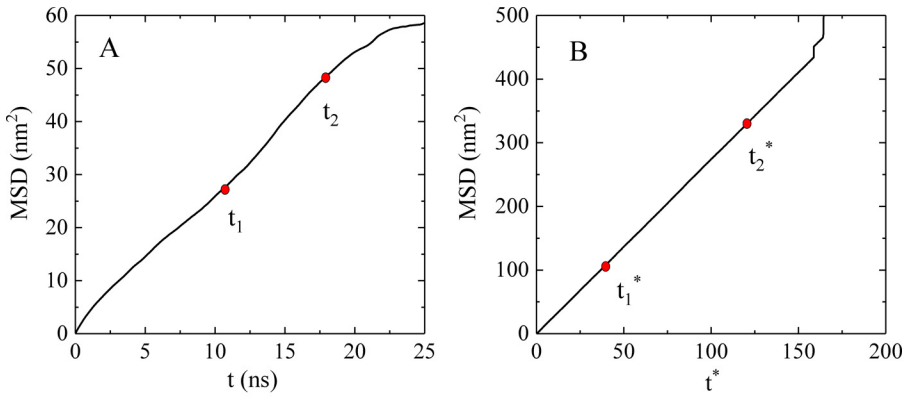

Fig. 11

Figure 11. Plots of the MSD *versus* time calculated from atomistic simulation (*A*) and DMD simulation (*B*). The two points are chosen from each of two plots to calculate the slope of MSD line *versus* time.