Supporting information

Adsorption of LRAP on Hydroxyapatite (001) Surface through $-COO^-$ Claws

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In order to obtain usable information from these SMD simulations, an observation window should be selected carefully. The spring constant should be weak enough to enhance the sensitivity of changes and strong enough to make LRAP follow the external force. If the pulling velocity were adjusted too fast, it would lose information regarding the relaxation of the protein. But on the other hand if it was too slow, it is hard to avoid the surrounding noise of water molecules. One reason is that LRAP, as the major component of functional segments of amelogenin, has quite loose and soft structure. To obtain this observation window in this work, a series of simulations on varied parameters were performed and the results were checked carefully in order to get converged results. First, the spring constant was fixed and the pulling velocity was changed to find a suited pulling velocity by comparing the force-time plot. Then an optimized velocity was fixed and the spring constant was adjusted to fit the system. Finally, both the pulling velocity and the spring constant were confirmed through the force-time plots. Some typical plots of these results are shown in Figs. S1 and S2. It shows in Fig. 1 that the profile of the curve changes from complicated to simple with the pulling velocity increasing. But as shown in Fig. S2, the curve becomes more complicated with the spring constant increasing. As a result, the spring constant k was set to be $30\,\text{kcal}\cdot\text{mol}^{-1}\cdot\text{Å}^{-2}$ and the pulling velocity was fixed at $5\times10^{-4}\,\text{Å}\cdot\text{fs}^{-1}$ to obtain good SMD observation window. We would like to point out that if this technical is performed to other systems, the converged parameters may be different and should be checked respectively.

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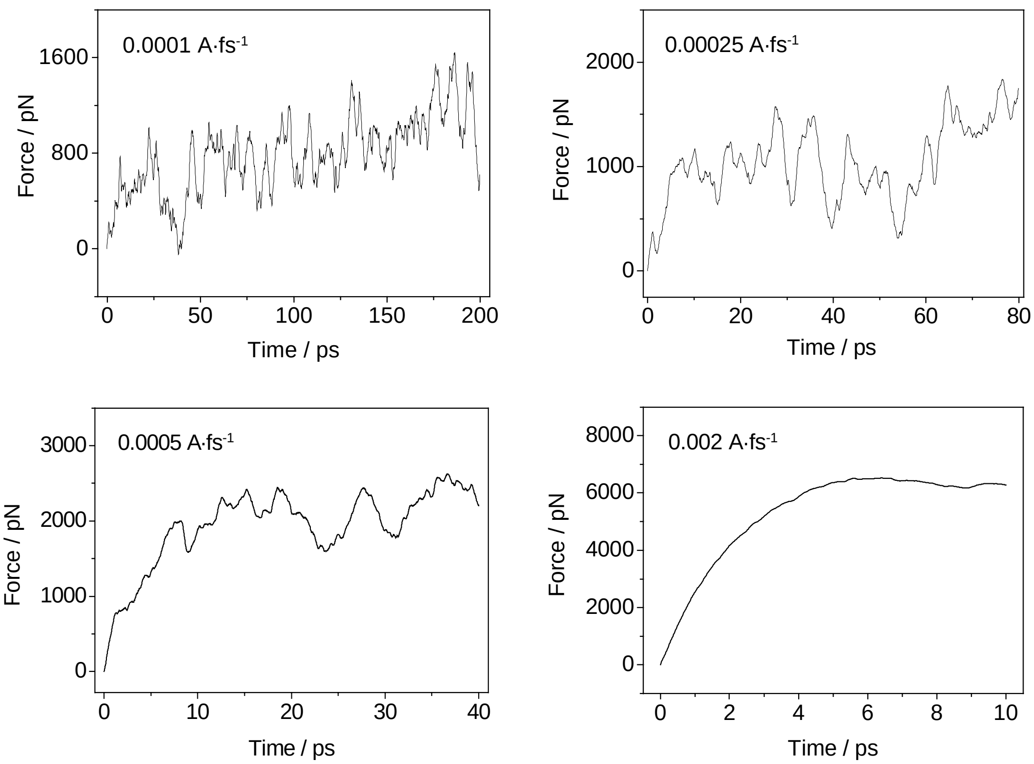

Fig. S1. Pulling force versus simulation time at different pulling velocities with the spring constant fixed. The spring constant *k* was fixed at 20 $\text{kcal}\cdot\text{mol}^{-1}\cdot\text{Å}^{-2}$ arbitrarily and the pulling velocities were set to be 0.0001, 0.00025, 0.0005 and 0.002 $\text{Å}\cdot\text{fs}^{-1}$, respectively. The pulling distance was set to be 20 Å, so the simulation time was different each other. The velocity of 0.0005 $\text{Å}\cdot\text{fs}^{-1}$ was chosen as the fixed pulling velocity for this system according to the complexity of these plots.

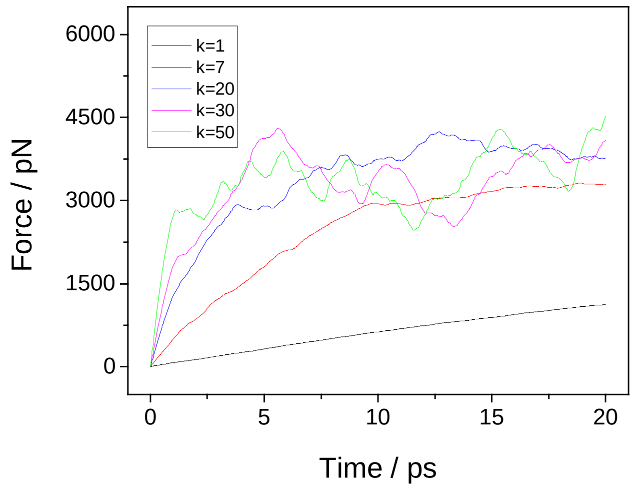

Fig. S2. Pulling force versus simulation time with different spring constants at fixed pulling velocity. The pulling velocity was fixed at 0.0005 $Å \cdot fs^{-1}$ and the spring constant was set to be 1, 7, 20, 30, and 50 $kcal \cdot mol^{-1} \cdot Å^{-2}$, respectively. The spring constant of 30 $kcal \cdot mol^{-1} \cdot Å^{-2}$ was chosen as the fixed *k* for this system according to the complexity of these curves.