**Table S3. MD parameter settings.** Parameters used for the MD equilibration and production phases.

|  |
| --- |
| **Relaxation Phase** |
|  | **Timestep** | **Numstep** | **Temperature** | **Harmonic Constraints****(kcal/(mol\*Å2))** | **Constant Temperature control** |
|  | ***Backbone*** | ***Sidechains*** | ***Lipids*** | ***Waters*** | ***Ions*** |  |
| ***Step1*** | 2.0 fs | 10 ns | 200 K | 10 | 10 | - | - | - | NPT |
| ***Step2*** | 2.0 fs | 10 ns | 300 K | - | - | - | - | - | NPT |
| **Production Phase** |
| ***Step1*** | 4.0 fs | 160 ns | 300 K | **-** | **-** | **-** | **-** | **-** | NPT |