**Supplementary File 3: Equilibration protocol for MD simulations**.

| Equilibration step | Time [$ps$] | Timestep $\left[ps\right]$ | Ensemble  | Thermostat | Barostat | Force constant backbone $\left[\frac{kJ}{molnm^{2}}\right]$ | Force constant side chain $\left[\frac{kJ}{molnm^{2}}\right]$ | Force constant lipids$\left[\frac{kJ}{molnm^{2}}\right]$ | Force constant dihedrals$\left[\frac{kJ}{molrad^{2}}\right]$ |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 1 | 125 | 0.001 | NVT | Berendsen |  | 4000 | 2000 | 1000 | 1000 |
| 2 | 125 | 0.001 | NVT | Berendsen |  | 2000 | 1000 | 400 | 400 |
| 3 | 125 | 0.001 | NPT | Berendsen | Berendsen (semi-isotropic) | 1000 | 500 | 400 | 200 |
| 4 | 500 | 0.002 | NPT | Berendsen | Berendsen (semi-isotropic) | 500 | 200 | 200 | 200 |
| 5 | 500 | 0.002 | NPT | Berendsen | Berendsen (semi-isotropic) | 200 | 50 | 40 | 100 |
| 6 | 500 | 0.002 | NPT | Berendsen | Berendsen (semi-isotropic) | 50 | 0 | 0 | 0 |