Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Modulation of Phase Transition of Thermosensitive Liposomes by Leucine Zipper-Structured Lipopeptides

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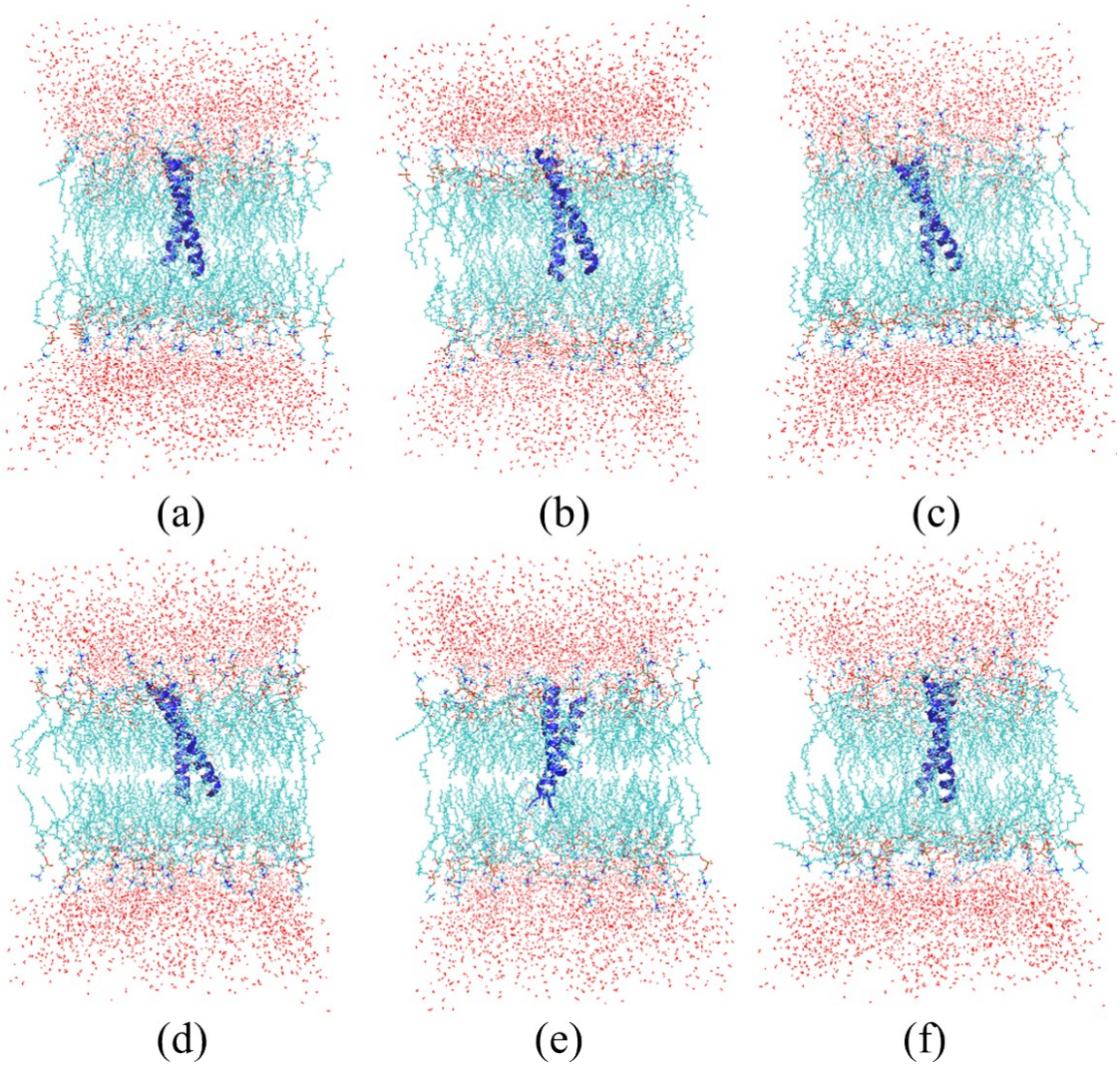



**Figure S1.** Initial structures of the six lipopeptide (a) ALA (b) C3CO (c) C5CO (d) C7CO (e) C7AS and (f) POCH dimers complexed with lipid DPPC bilayer and water.

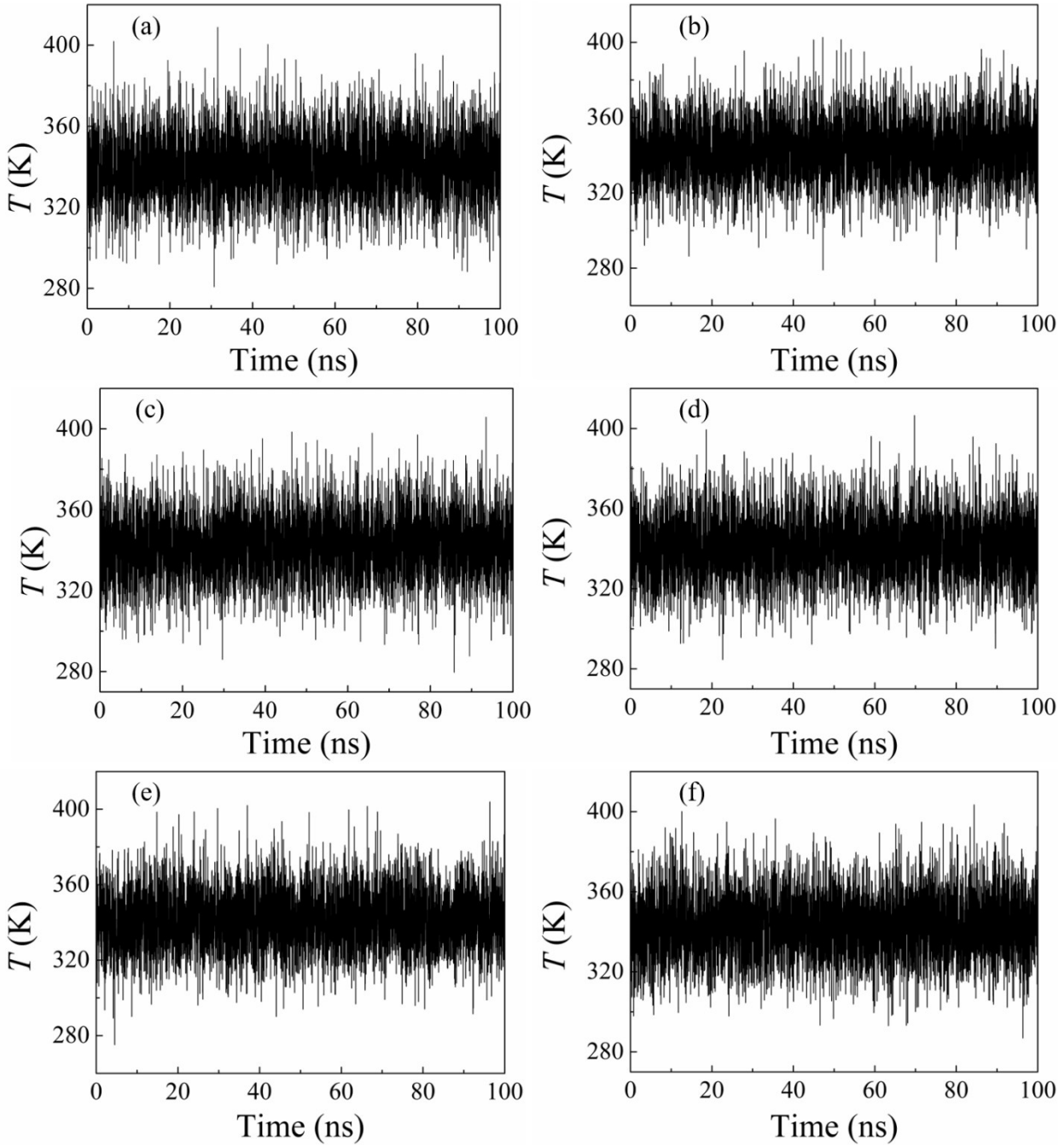



**Figure S2.** Time series of temperature exchanges for replica 8. (a) ALA (b) C3CO (c) C5CO (d) C7CO (e) C7AS and (f) POCH lipopeptides.

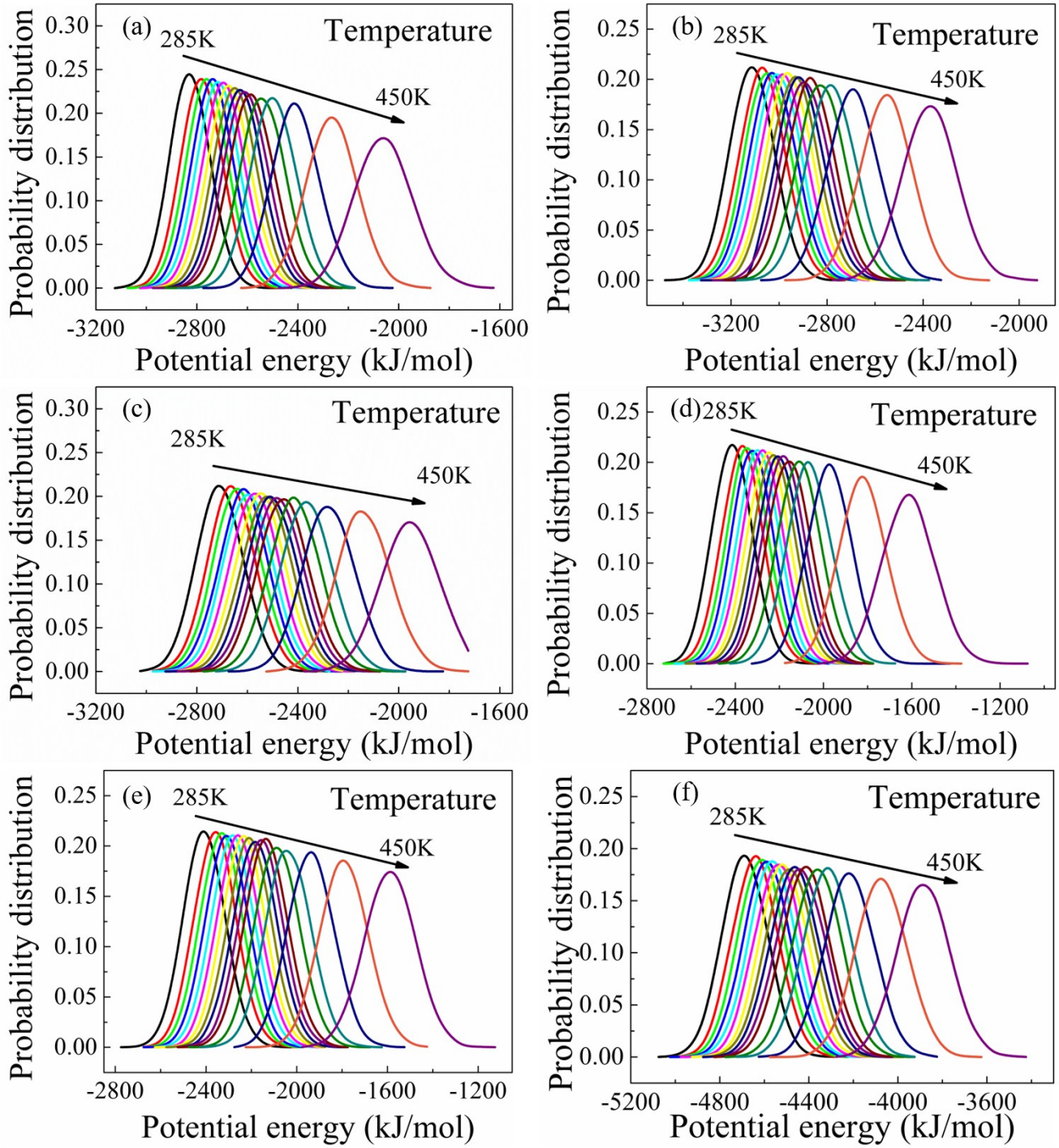
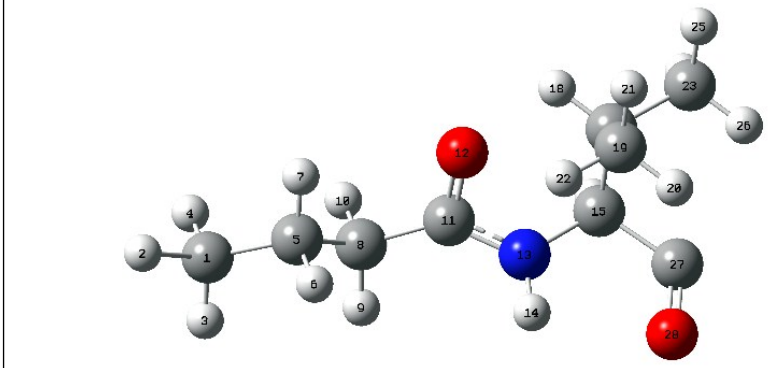
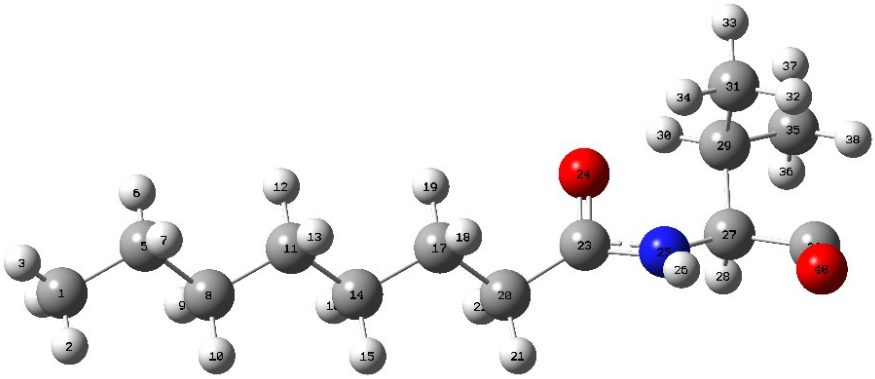



**Figure S3.** The probability distributions of the potential energy of the replicas at the temperatures: 285 K, 295 K, 300 K, 305 K, 310 K, 315 K, 320 K, 325 K, 330 K, 335 K, 340 K, 350 K, 360 K, 380 K, 410 K and 450 K. REMD simulations for the (a) ALA (b) C3CO (c) C5CO (d) C7CO (e) C7AS and (f) POCH lipopeptides.

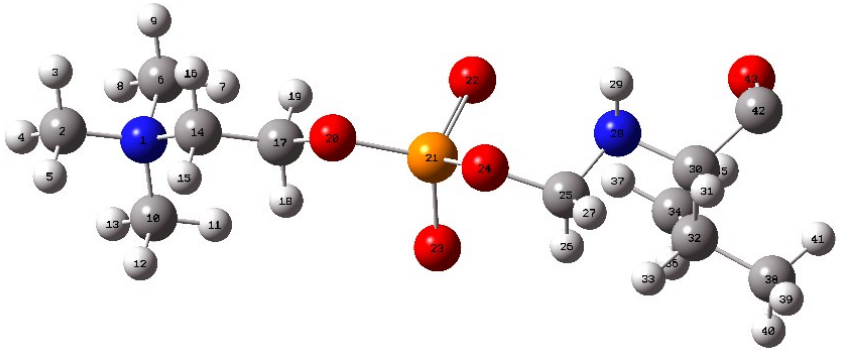
**Table S1.** Derived partial charges of the head groups capped in the lipopeptides C3CO, C7CO/C7AS, and POCH.

| C3CO |  |
|---|---|

| Index of the atom | Partial charges | Index of the atom | Partial charges | Index of the atom | Partial charges |
|---|---|---|---|---|---|
| 1 | 0.0665 | 5 | 0.4968 | 9 | 0.4705 |
| 2 | 0.0102 | 6 | -0.0604 | 10 | 0.4705 |
| 3 | 0.0102 | 7 | -0.0604 | 11 | 2.0105 |
| 4 | 0.0102 | 8 | -1.9082 | 12 | -0.5164 |

| C7CO/ C7AS |  |
|---|---|

| Index of the atom | Partial charges | Index of the atom | Partial charges | Index of the atom | Partial charges |
|---|---|---|---|---|---|
| 1 | -0.3866 | 9 | 0.0029 | 17 | 0.1523 |
| 2 | 0.1101 | 10 | 0.0029 | 18 | -0.0038 |
| 3 | 0.1101 | 11 | -0.4098 | 19 | -0.0038 |
| 4 | 0.1101 | 12 | 0.0873 | 20 | -1.1160 |
| 5 | 0.2643 | 13 | 0.0873 | 21 | 0.2450 |
| 6 | -0.0169 | 14 | 0.4373 | 22 | 0.2450 |
| 7 | -0.0169 | 15 | -0.0319 | 23 | 1.5527 |
| 8 | 0.0308 | 16 | -0.0319 | 24 | -0.4205 |

| POCH |  |
|---|---|

| Index of the atom | Partial charges | Index of the atom | Partial charges | Index of the atom | Partial charges |
|---|---|---|---|---|---|
| 1 | 0.2264 | 10 | -0.3836 | 19 | 0.0117 |
| 2 | -0.3836 | 11 | 0.1908 | 20 | -0.4083 |
| 3 | 0.1908 | 12 | 0.1908 | 21 | 1.1288 |
| 4 | 0.1908 | 13 | 0.1908 | 22 | -0.6772 |
| 5 | 0.1908 | 14 | -0.6869 | 23 | -0.6772 |
| 6 | -0.3836 | 15 | 0.2806 | 24 | -1.0904 |
| 7 | 0.1908 | 16 | 0.2806 | 25 | 2.5849 |
| 8 | 0.1908 | 17 | 0.4781 | 26 | -0.5146 |
| 9 | 0.1908 | 18 | 0.0117 | 27 | -0.5146 |

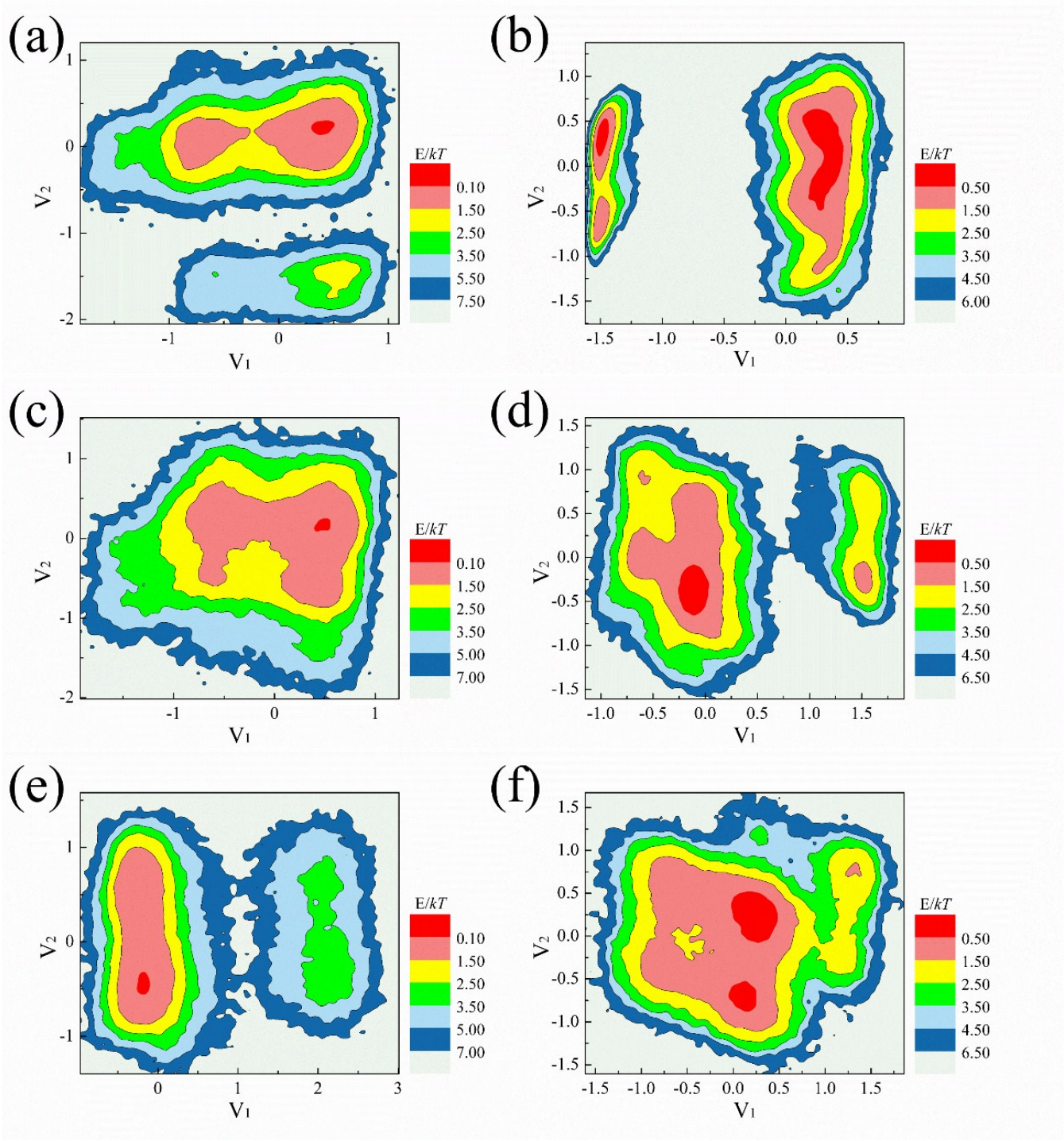



**Figure S4.** Free energy landscape ($\varphi$) along the first two principal components ($V_1$, $V_2$) for the lipopeptide C7CO at (a) 305 K, (c) 350 K and (e) 410 K, and for the lipopeptide C7AS at (b) 305 K, (d) 350 K and (f) 410 K. The unit of FEL is *kT*.

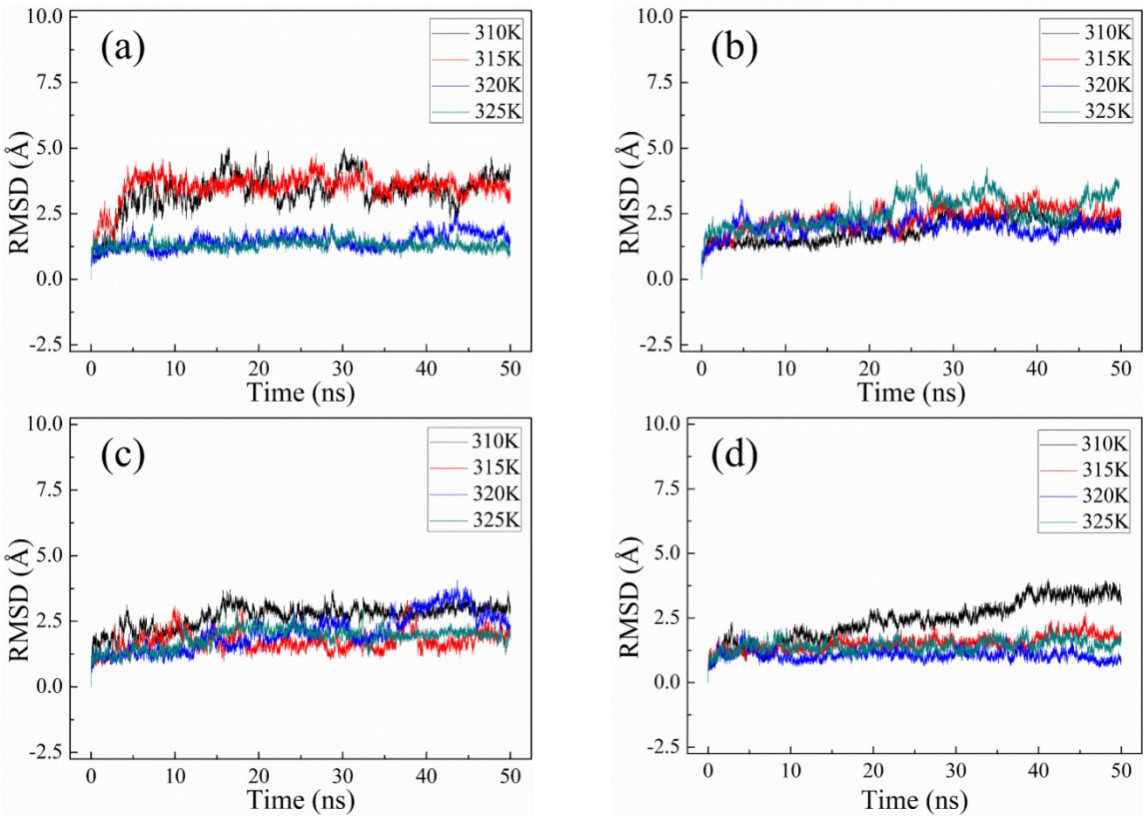



**Figure S5.** The RMSD profiles of the lipopeptide dimers (a) ALA, (b) C3CO, (c) C5CO and (d) POCH in the 50-ns conventional MD simulations at 310 K, 315 K, 320 K and 325 K.

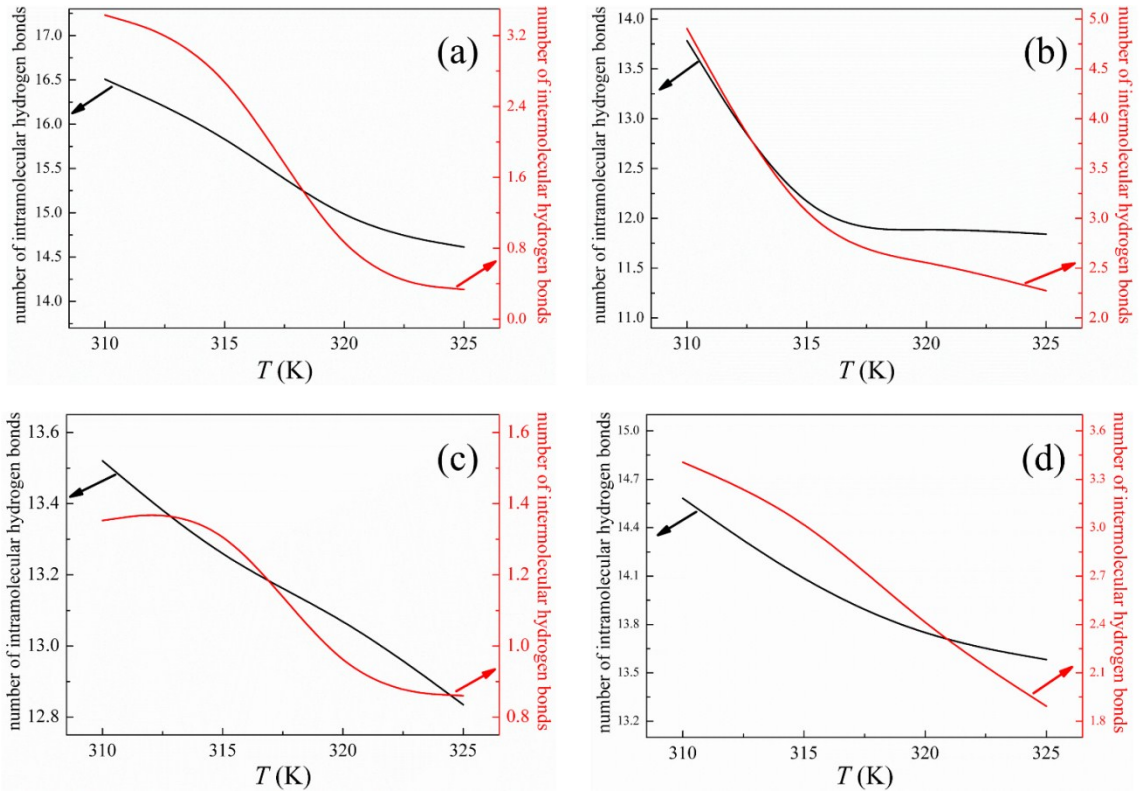



**Figure S6.** The effect of temperature on the intramolecular and intermolecular hydrogen bonds for the lipopeptide dimers (a) ALA, (b) C3CO, (c) C5CO, and (d) POCH.