|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| # of Tat | AL | ZTat | <DPP> | DPP | x | ∆t | R2 | ZPhos | Zguanidinium | χ2 |
| 0 (DOPC) | 70 | NA | 36.3 | NA | NA | NA | NA | NA | NA | NA |
| 2 | 72 | 18 | 35.6 | 32.8 | 35.8 | 3.5 | 15.0 | 14.7 | 15.5 | 18 |
| 2 | 72 | 16 | 36.1 | 33.0 | 36.3 | 3.3 | 9.0 | 14.9 | 14.5 | 24.9 |
| 2 | 74 | 18 | 35.0 | 33.0 | 35.1 | 3.3 | 23.9 | 14.9 | 16.5 | 21.3 |
| 2 | 74 | 16 | 35.0 | 32.1 | 35.2 | 4.2 | 20.4 | 14.0 | 13.5 | 25.9 |
| 4 | 74 | 18 | 35.3 | 32.6 | NA | 3.7 | NA | 14.5 | 15.5 | 24.3 |
| 4 | 74 | 16 | 35.3 | 31.2 | NA | 5.1 | NA | 13.1 | 13.5 | 40.1 |
| 4 | 76 | 18 | 34.2 | 32.0 | NA | 4.3 | NA | 13.9 | 16.5 | 14.8 |
| 4 | 76 | 16 | 34.9 | 31.4 | NA | 4.9 | NA | 13.3 | 14.5 | 30.4 |

AL: area per lipid defined as simulation area divided by 64, the number of lipids in a leaflet

ZTat: constrained center of mass of Tat along Z-axis

<DPP>: phosphorus-phosphorus distance averaged over all lipids, can be directly obtained from SIMtoEXP

DPP: local phosphorus-phosphorus distance, defined to be within the Tat cylinder (R=9 Å), mined from simulation trajectories

x = (64\*<DPP> – 3.5\*DPP) / 60.5 = thickness away from Tat

∆t = <DPP0> – DPP, where <DPP0> is the value from the DOPC simulation (=36.3)

Zguanidinium was defined as the peak position of the distribution. Should we also calculate the mean of the distribution? (Probably no because some of the guanidinium groups are in water)

ZP = DPP – <DPP0> / 2

x and R2 were not calculated for 4 Tat simulations because Tat-cylinders on the same leaflet could overlap, complicating the calculations

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| # of Tat | AL | ZTat | <DPP> | DPP | x | ∆t | R2 | ZPhos | Zguanidinium |
| 2 | 72.9 | 17.1 | 35.4 | 32.7 | 35.6 | 3.6 | 17.1 | 14.6 | 15.1 |
| 4 | 75.2 | 17.3 | 34.8 | 31.9 | NA | 4.4 | NA | 13.8 | 15.4 |