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

Supporting Information for

Simulation study of domain formation in a model bacterial membrane

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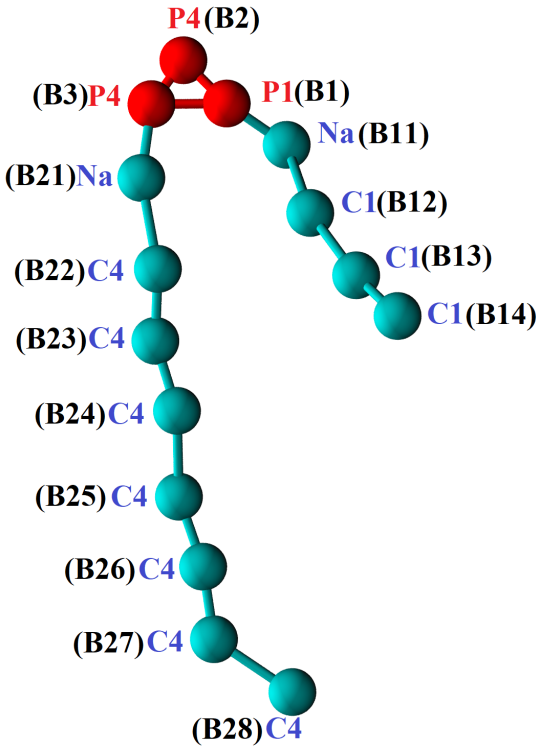


Figure S1: Coarse-grained representation of the STX molecule. Red and cyan color represent head and tail beads of the STX molecule, respectively. Bead name along with the MARTINI bead type are also shown in the figure.

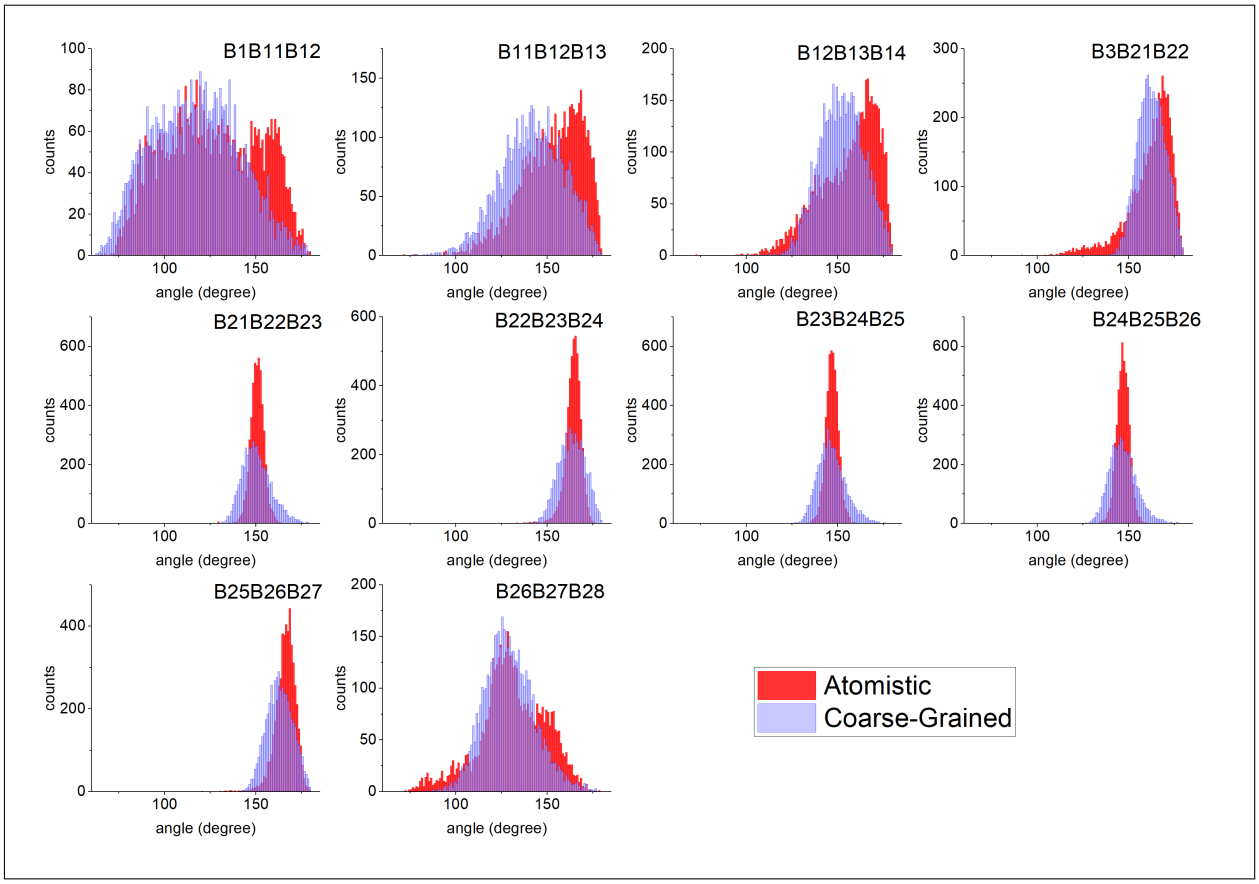


Figure S2: Distributions of different angles obtained from the atomistic and coarse-grained simulations. Red and blue color represent atomistic and coarse-grained results, respectively.

Table 1: Summary of the simulations performed in this study

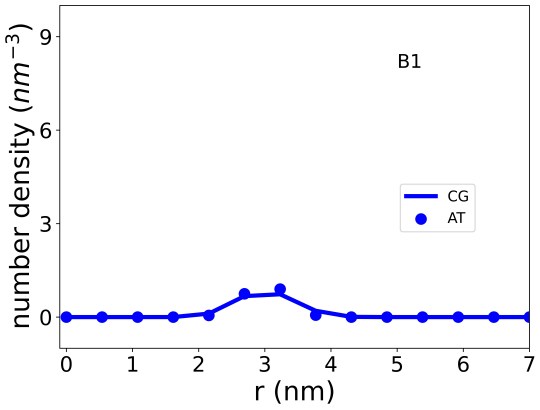
System	Number of lipids	DPPG(%)	CDL(%)	STX(%)	Total number of atoms/beads	Simulation time(μs)
Single STX in solution (AT)	1	-	-	100	20973	0.1
Single STX in solution (CG)	1	-	-	100	979	0.5
Micelle in solution (AT)	103	-	-	100	140615	0.1
Micelle in solution (CG)	103	-	-	100	16191	1
5% STX membrane	4000	80	15	5	135234	20
10% STX membrane	4000	75	15	10	135103	20
20% STX membrane	4000	65	15	20	131443	20
FloA protein + membrane	4000	75	15	10	176970	10
PBP2a protein + membrane	4000	75	15	10	160064	20
Domain disassembly	4000	75	15	10	132303	4
Domain disassembly with PBP2a	4000	75	15	10	157264	2
Domain without B2 bead	1000	65	15	20	26089	10

Table 2: Bond parameters of the CG model of STX.

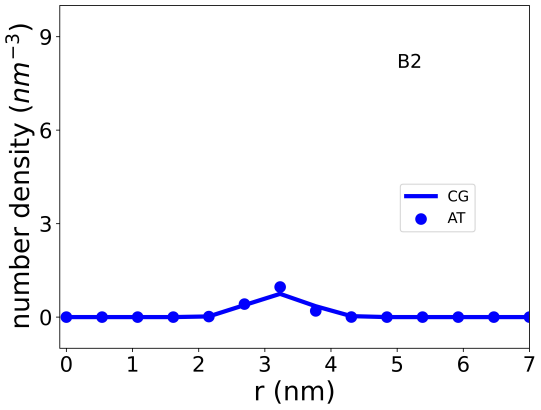
bonds	mean bonglength (nm)	force constant $(kJmol^{-1}nm^{-2})$
B1-B11	0.375	1800
B3-B21	0.367	7000
B11-B12	0.435	2000
B12-B13	0.475	3000
B13-B14	0.385	3500
B21-B22	0.422	30000
B22-B23	0.333	30000
B23-B24	0.333	30000
B24-B25	0.435	28000
B25-B26	0.331	25000
B26-B27	0.327	12000
B27-B28	0.415	12000

Table 3: Angle parameters of the CG model of STX.

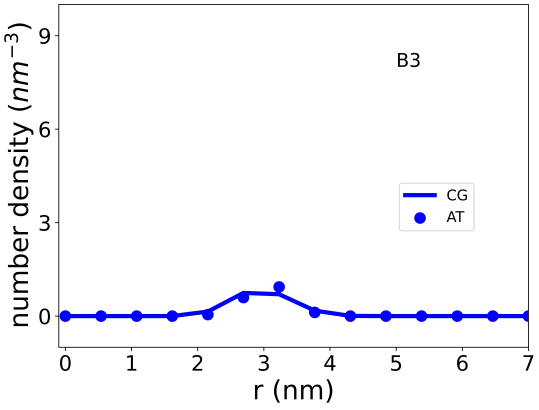
angles	mean angle $(^o)$	force constant $(kJmol^{-1}nm^{-2})$
B1-B11-B12	115	3.0
B11-B12-B13	190	22.0
B12-B13-B14	190	100.0
B3-B21-B22	180	620.0
B21-B22-B23	151	500.0
B22-B23-B24	180	700.0
B23-B24-B25	147	500.0
B24-B25-B26	147	500.0
B25-B26-B27	180.5	700.0
B26-B27-B28	130.5	75.0



(a)

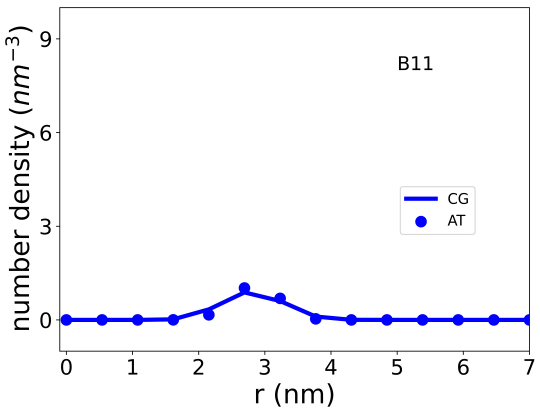


(b)

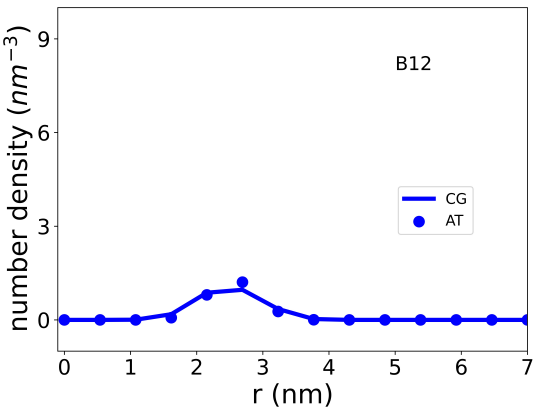


(c)

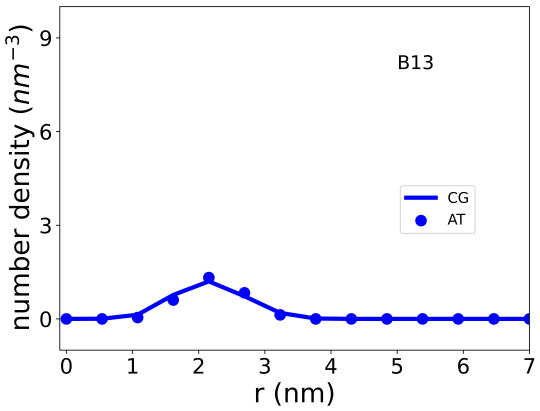
Figure S3: Comparison between number densities of different head beads obtained from atomistic and coarse-grained simulations.


B11
CG
AT
number density (nm^{-3})
r (nm)
0
3
6
9
0
1
2
3
4
5
6
7

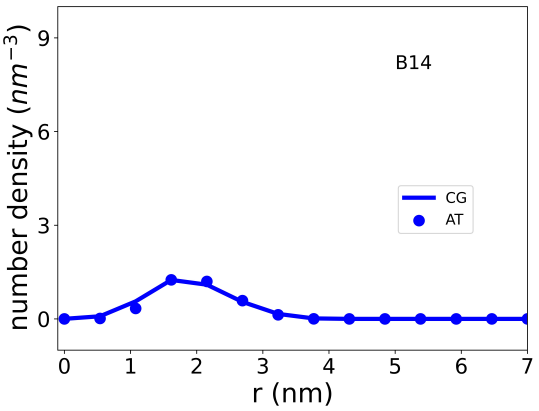
(a)


B12
CG
AT
number density (nm^{-3})
r (nm)
0
3
6
9
0
1
2
3
4
5
6
7

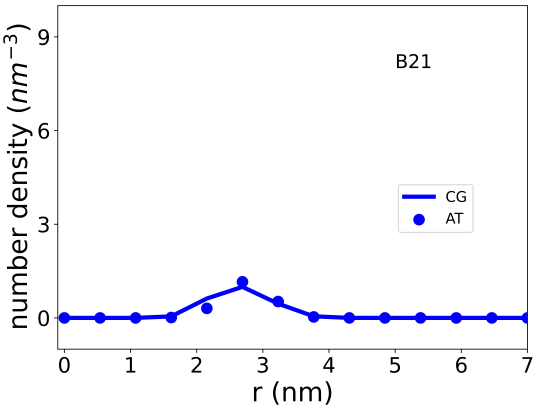
(b)


B13
CG
AT
number density (nm^{-3})
r (nm)
0
3
6
9
0
1
2
3
4
5
6
7

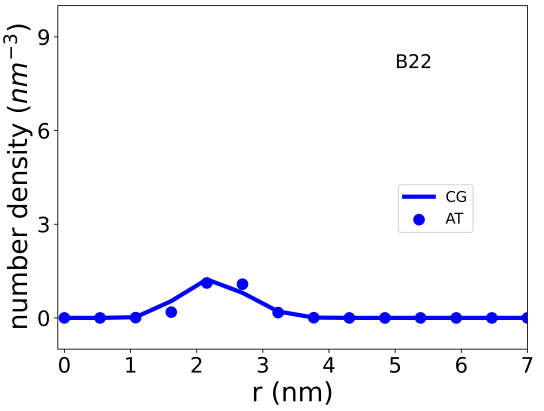
(c)


B14
CG
AT
number density (nm^{-3})
r (nm)
0
3
6
9
0
1
2
3
4
5
6
7

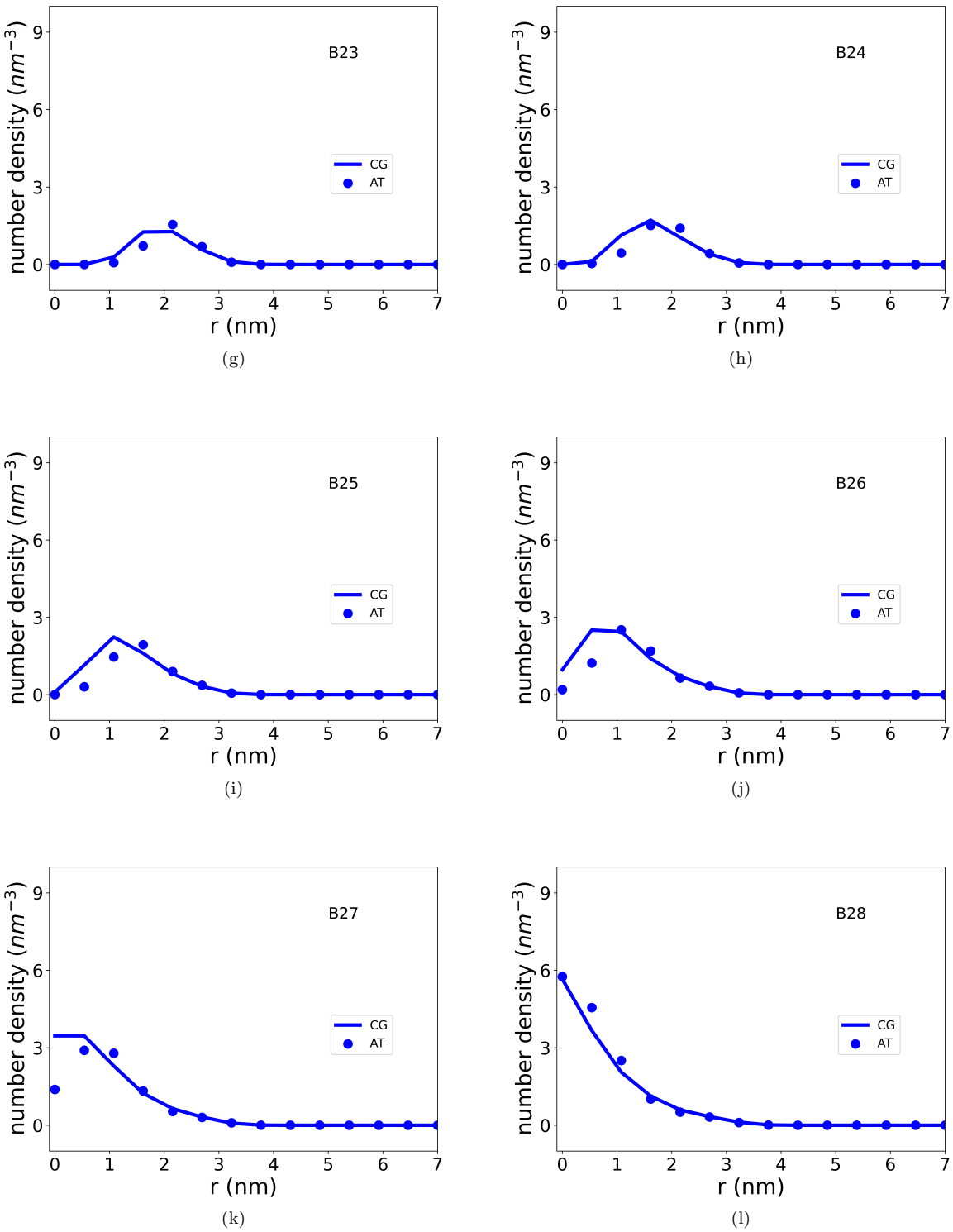
(d)


B21
CG
AT
number density (nm^{-3})
r (nm)
0
3
6
9
0
1
2
3
4
5
6
7

(e)


B22
CG
AT
number density (nm^{-3})
r (nm)
0
3
6
9
0
1
2
3
4
5
6
7

(f)



(g) (h) (i) (j) (k) (l)

Figure S4: Comparison between number densities of different tail beads obtained from atomistic and coarse-grained simulations.

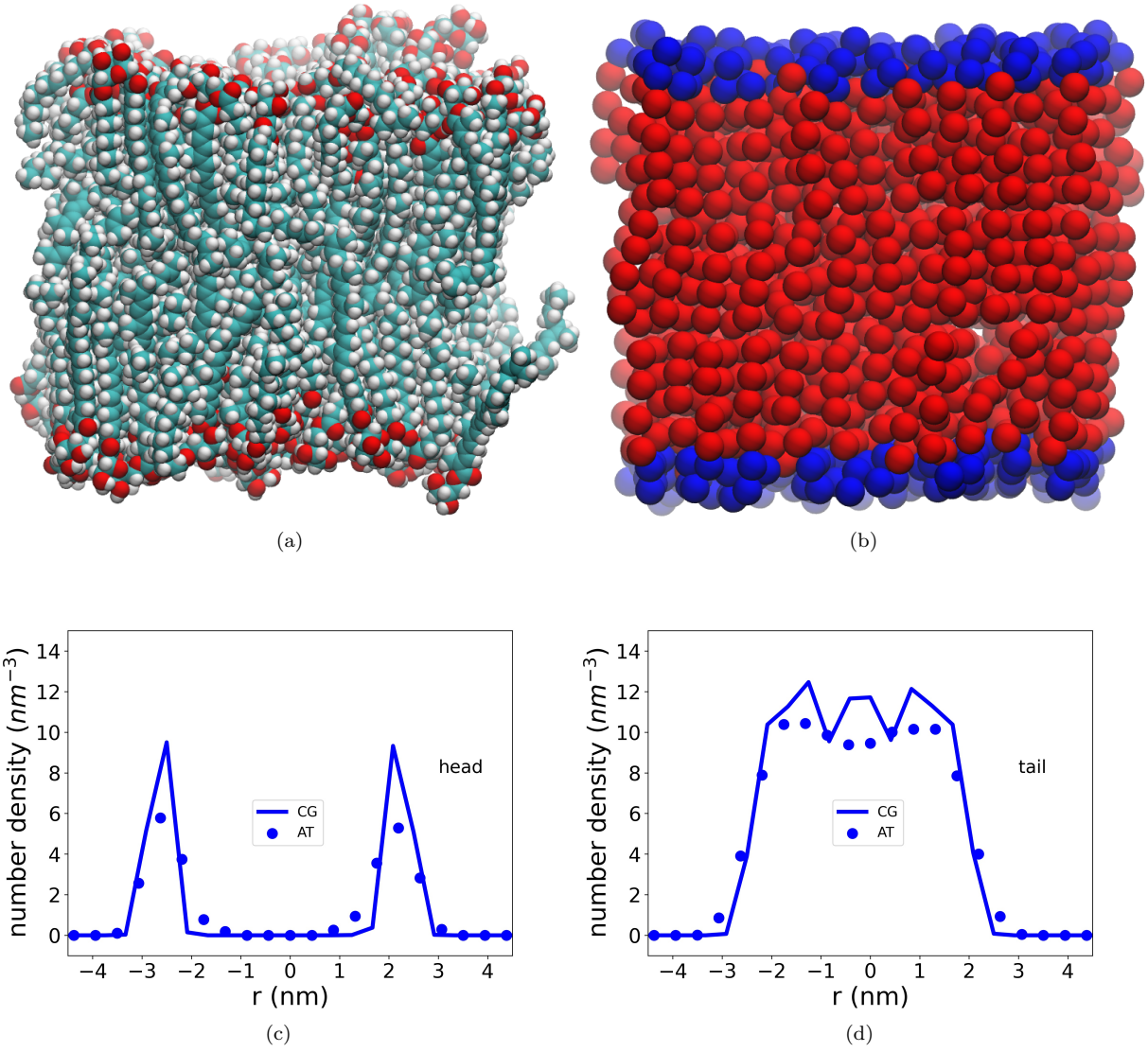
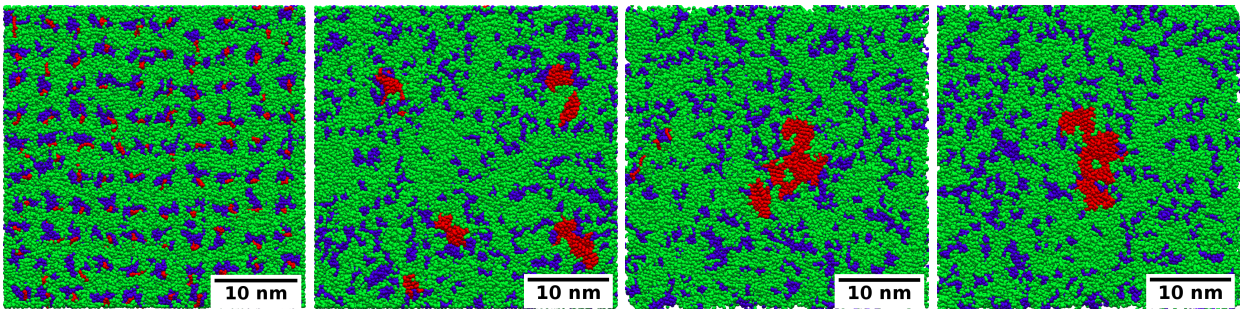
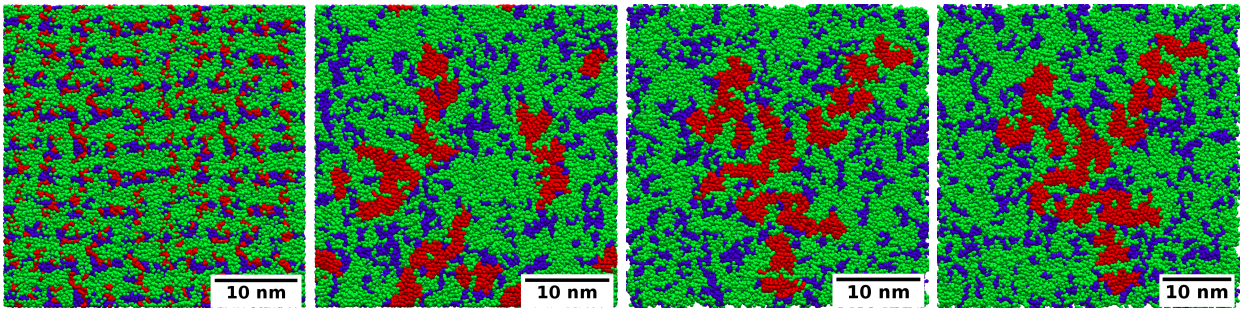


Figure S5: Equilibrated structure of STX bilayer simulated using (a) atomistic and (b) coarse-grained model. Red, cyan and white color in the atomistic structure represent oxygen, carbon and, hydrogen, respectively. Blue and red color in the coarse-grained structure represent head and tail of the STX, respectively. Water and ions are removed for better visibility. Comparison of the (c) head and (d) tail density of the STX molecule obtained from the atomistic and coarse-grained simulations.



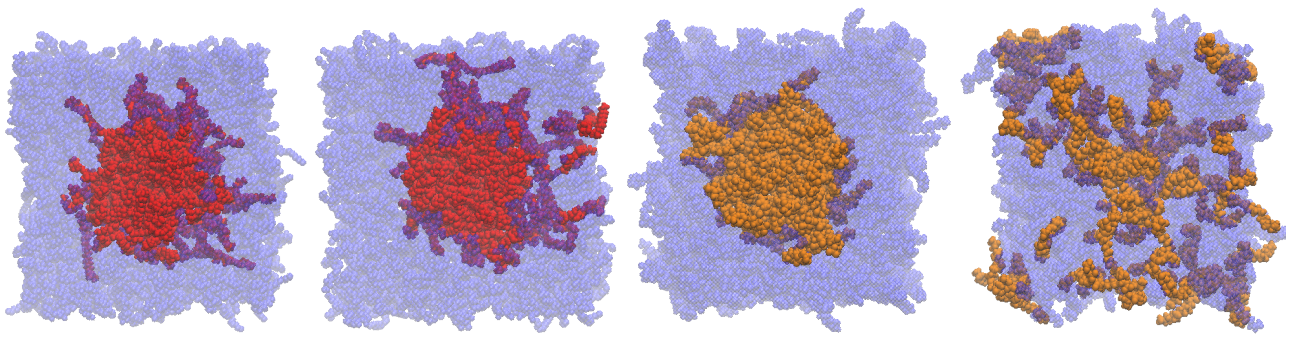
(a) (b) (c) (d)

Figure S6: Top view of the instantaneous structure of the mixed lipid bilayer containing 5% STX at (a) 0 μs, (b) 1.5 μs, (c) 10 μs and (d) 20 μs. Green, blue, and red colors represent DPPG, CDL and STX lipids, respectively. Water and ion beads are removed for clarity.



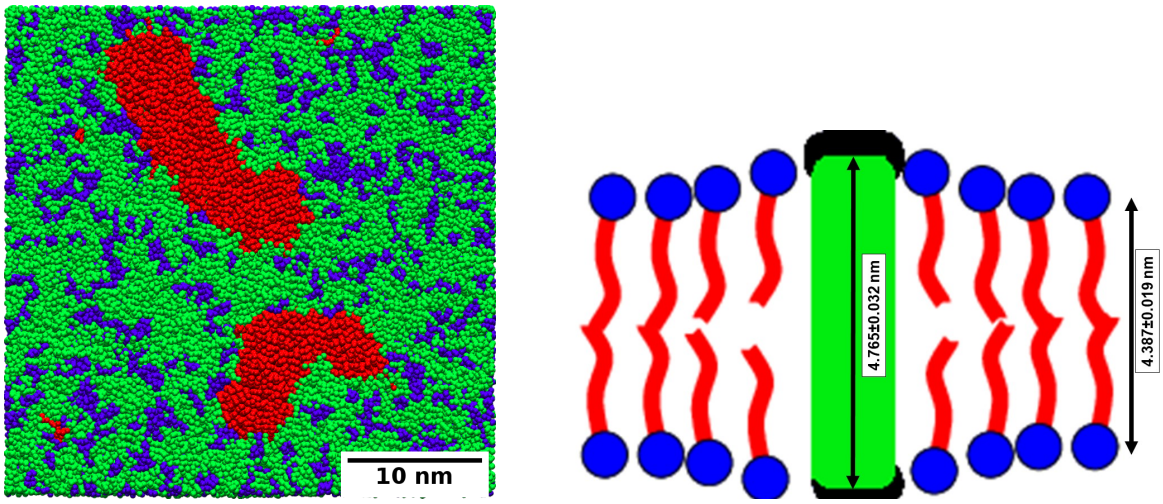
(a) (b) (c) (d)

Figure S7: Top view of the instantaneous structure of the mixed lipid bilayer containing 20% STX at (a) 0 μs, (b) 1.5 μs, (c) 10 μs and (d) 20 μs. Green, blue, and red colors represent DPPG, CDL and STX lipids, respectively. Water and ion beads are removed for clarity.



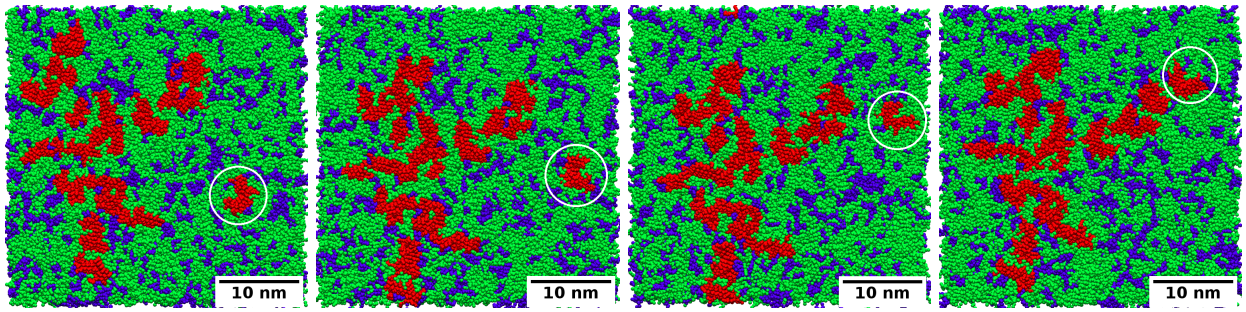
(a) (b) (c) (d)

Figure S8: (a) An STX cluster (red) is initially inserted in a DPPG/CDL (transparent blue) mixed lipid bilayer. (b) Final structure of the system obtained after 500 ns long simulation. The STX cluster maintains its integrity. (c) Yellow color represents the DPPG/CDL lipids initially near the center of a DPPG/CDL mixed lipid bilayer which are randomly dispersed after only 250 ns long simulation (d). Water and ions are removed for better visibility.



(a) (b)

Figure S9: (a) Phase separated structure obtained with a 'symmetric' STX molecule. The last four beads of the bigger STX tail are removed and all the tail beads of STX are set to 'C4' type to make the two tails of STX chemically and structurally symmetric (see text for details). An initial structure containing randomly mixed symmetric STX (20%) and DPPG/CDL lipids is solvated and energy minimized. The final structure obtained after $10\mu s$ long simulation is shown in (a). (b) A schematic figure showing that the STX cluster (green and black) is thicker than the DPPG/CDL mixture (red and blue). Hydrophobic mismatch at the STX-DPPG/CDL boundary creates a local membrane curvature.



(a) (b) (c) (d)

Figure S10: Representative snapshots at around (a) 6.5 (b) 7.6 (c) 7.9 and (d) 9.0 μs showing a small STX cluster, marked by the white circle, gradually migrating to the STX-rich domain in the 20% STX system.

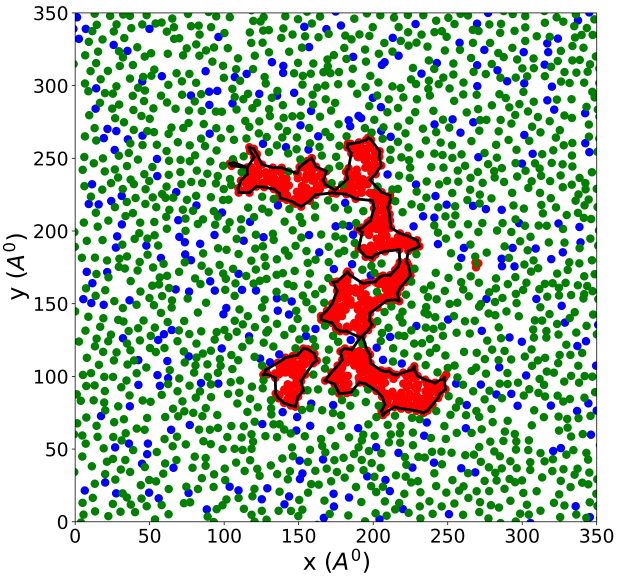
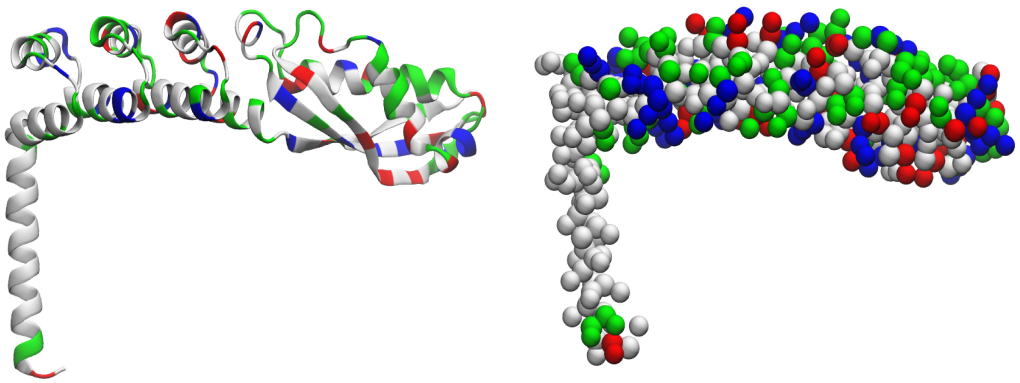
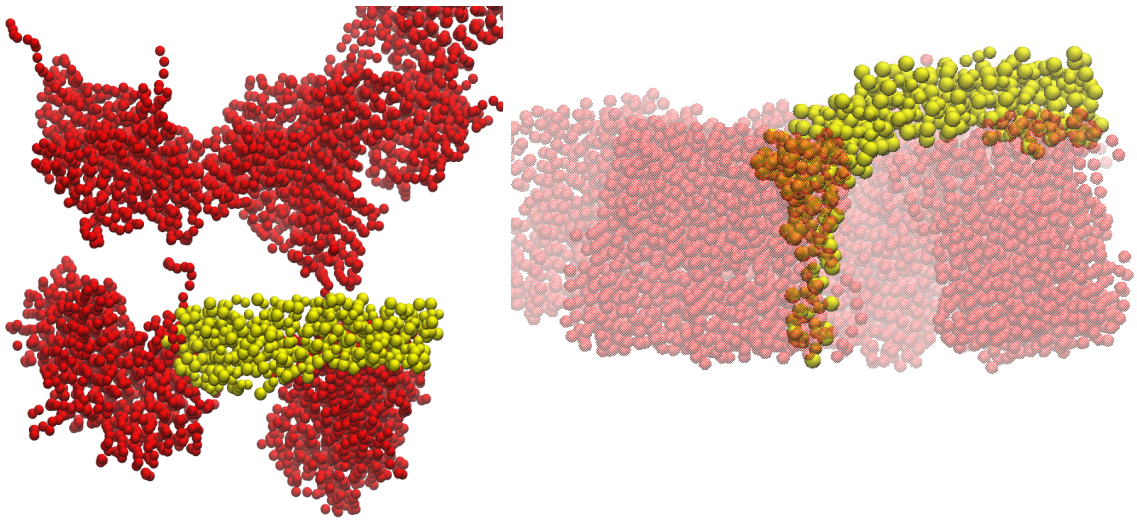


Figure S11: Black line shows an instantaneous interfacial boundary between the STX domain and DPPG/CDL mixture. Green and blue dots represent PO4 beads of DPPG and CDL, respectively. Red color represents the STX domain.



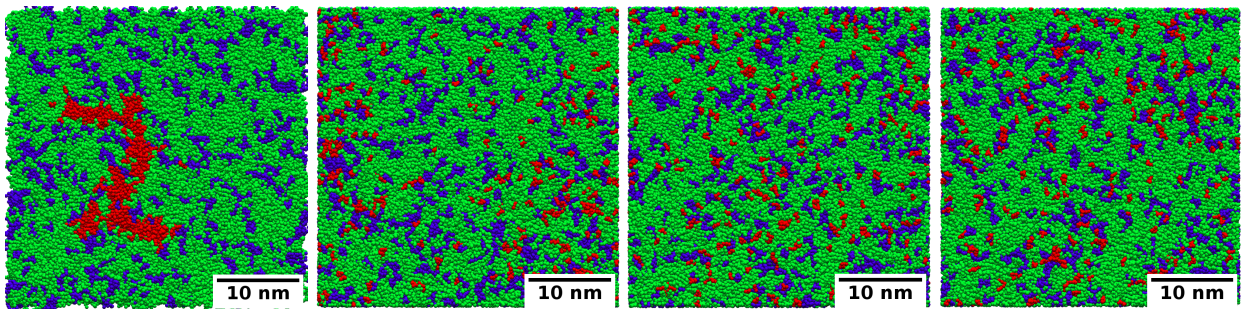
(a) (b)

Figure S12: (a) Atomistic and (b) Coarse-grained representation of the N-terminal domain of floA protein.



(a) (b)

Figure S13: (a) Top and (b) side view of zoom-in figures showing floA protein preferentially binds with the STX domain. Red and yellow color represent STX and N-terminal domain of the floA protein, respectively.



(a) (b) (c) (d)

Figure S14: Top view of the instantaneous structure of a membrane domain from which the STX unsaturated tails are truncated, at (a) 0 μs, (b) 0.5 μs, (c) 2 μs and (d) 4 μs. Green, blue, and red colors represent DPPG, CDL and STX lipids, respectively. Water and ion beads are removed for clarity.