Supplemental information

A new lipid force field (FUJI)

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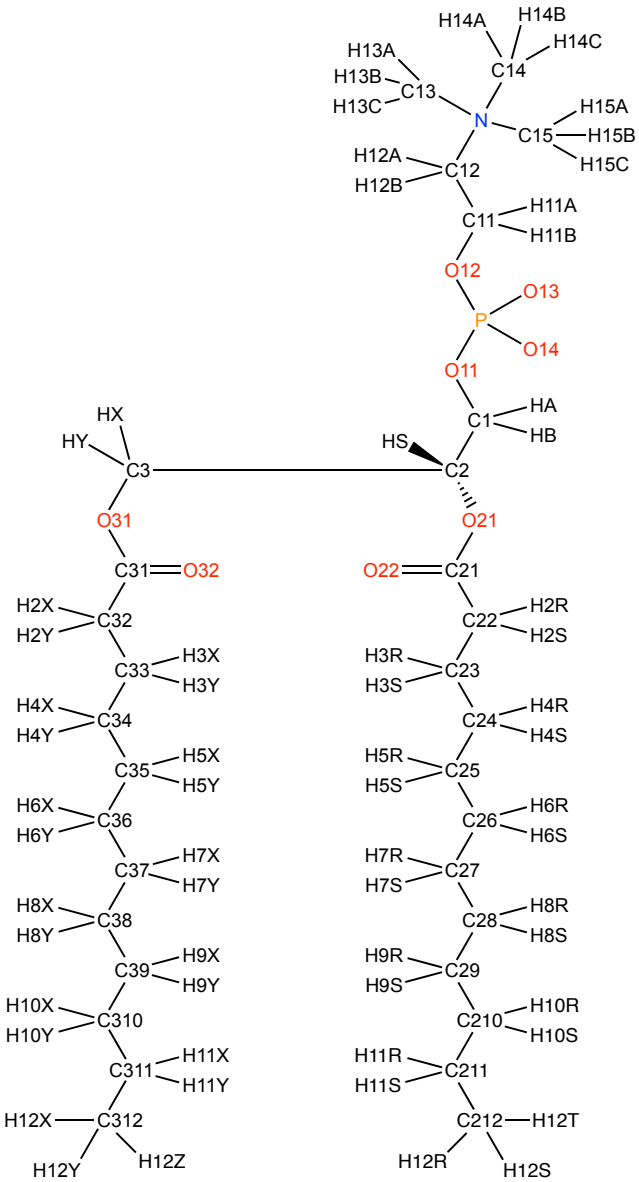

Figure S1: Molecular structure and atomic names of dilauroyl-phosphatidyl-choline (DLPC).

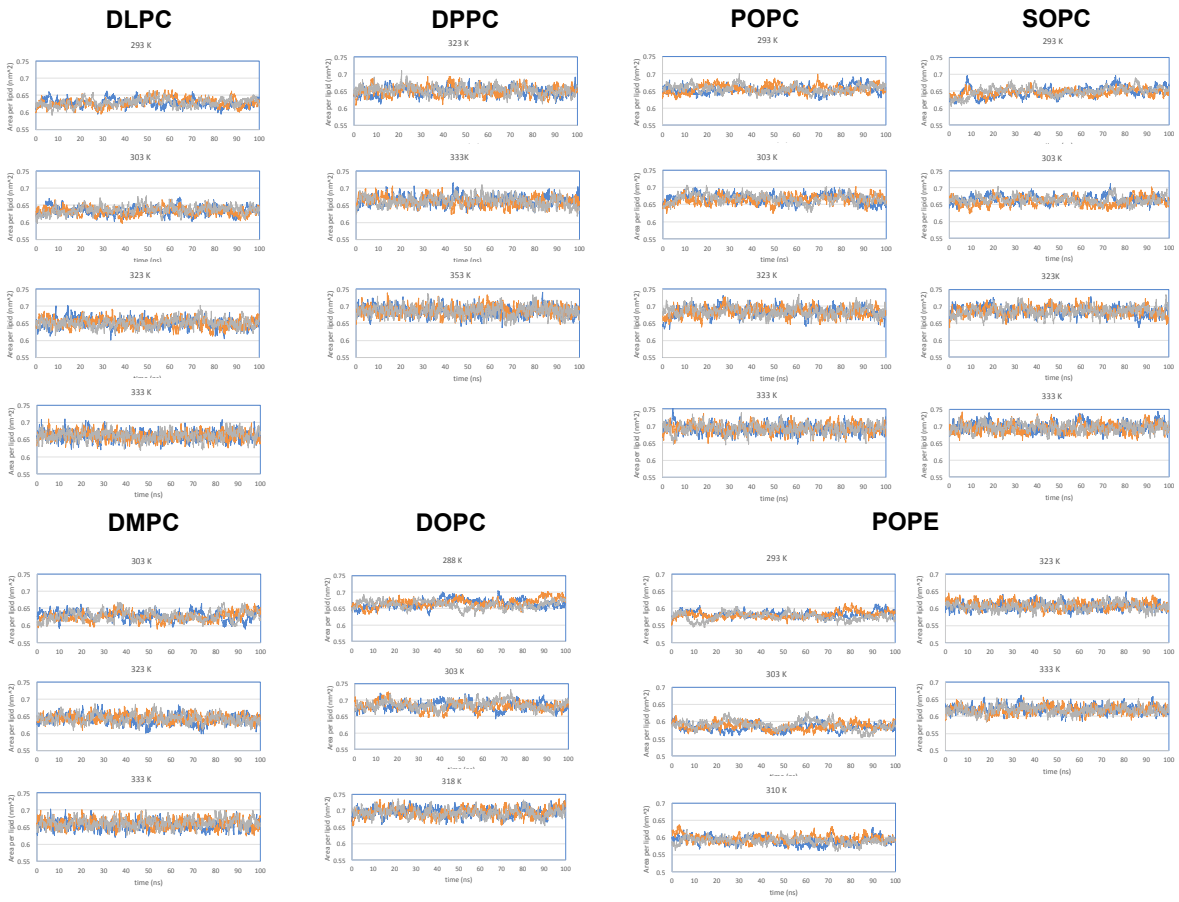

Figure S2: Time evolution of area per lipid for the seven lipid bilayers at the lowest simulation temperature. The results of three runs are shown in different colors.

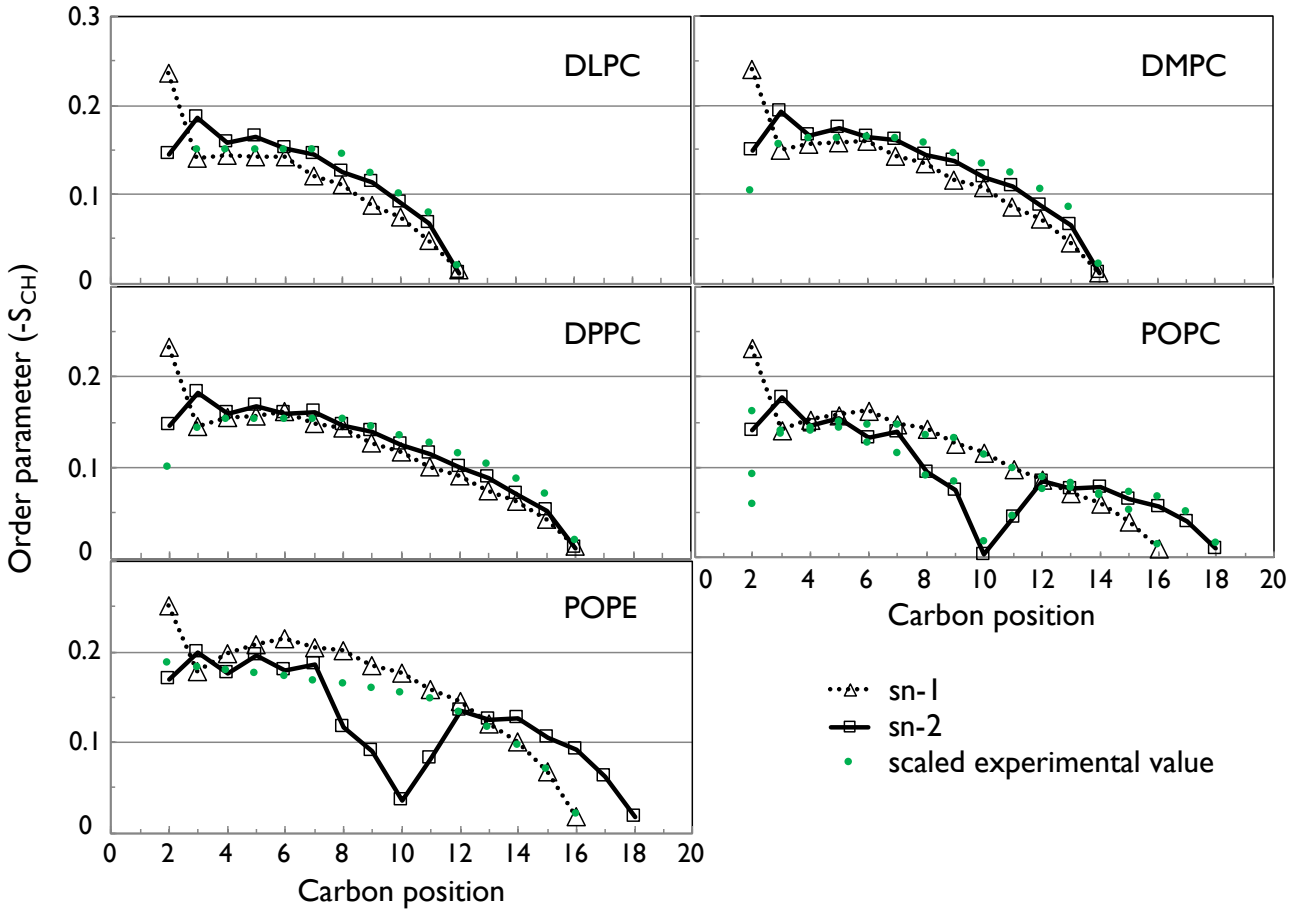

Figure S3: Order-parameter profiles for the acyl tails with experimental values scaled by 0.7 (DLPC, DMPC, DPPC, and POPE) and by 0.75 (POPC).

Table S1: Point charges and atom types in the lipid head parts.

Phosphatidylcholine (PC)			Phophatidylethanolamine (PE)		
Atom name	Atom type	Charge	Atom name	Atom type	Charge
N	N4x	0.0651	N	N4x	-0.3574
C13	C3	-0.0744	HN1	HN	0.3246
H13A	HX	0.0854	HN2	HN	0.3246
H13B	HX	0.0854	HN3	HN	0.3246
H13C	HX	0.0854	C12	C3	0.0129
C14	C3	-0.0744	H12A	HX	0.0896
H14A	HX	0.0854	H12B	HX	0.0896
H14B	HX	0.0854	C11	C3	0.1706
H14C	HX	0.0854	H11A	H1	0.0457
C15	C3	-0.0744	H11B	H1	0.0457
H15A	HX	0.0854	P	P5	1.3181
H15B	HX	0.0854	O13	OPx	-0.8123
H15C	HX	0.0854	O14	OPx	-0.8123
C12	C3	0.0216	O12	OTx	-0.5109
H12A	HX	0.0612	O11	OTx	-0.4453
H12B	HX	0.0612	C1	C3	0.0726
C11	C3	0.2829	HA	H1	0.0849
H11A	H1	-0.0073	HB	H1	0.0849
H11B	H1	-0.0073	C2	C3	0.0757
P	P5	1.2033	HS	H1	0.1415
O13	OPx	-0.7774	O21	OSx	-0.4078
O14	OPx	-0.7774	C21	Cox	0.7815
O12	OTx	-0.4425	O22	Ox	-0.6277
O11	OTx	-0.4108	C22	CTx	-0.0492
C1	C3	0.0721	H2R	HCx	0.0307
HA	H1	0.0786	H2S	HCx	0.0307
HB	H1	0.0786	C3	C3	0.0005
C2	C3	0.0740	HX	H1	0.1200
HS	H1	0.1427	HY	H1	0.1200
O21	OSx	-0.4038	O31	OSx	-0.4578
C21	Cox	0.7734	C31	Cox	0.7985
O22	Ox	-0.6233	O32	Ox	-0.6211
C22	CTx	-0.0455	C32	CTx	-0.0435
H2R	HCx	0.0305	H2X	HCx	0.0280
H2S	HCx	0.0305	H2Y	HCx	0.0280
C3	C3	-0.0054			
HX	H1	0.1225			
HY	H1	0.1225			
O31	OSx	-0.4584			
C31	Cox	0.7971			
O32	Ox	-0.6193			
C32	CTx	-0.0440			
H2X	HCx	0.0287			
H2Y	HCx	0.0287			

Table S2: Point charges in the lipid tail parts. sp3 carbon atoms have the CTx atom type, to which the hydrogen atoms of the HCx atom type are connected. The sp2 carbon atoms of C29 and C210 in oleoyl have the C2 atom type, to which the hydrogen atoms of the HAx atom type are connected.

Lauroyl (LA)		Myristoyl (MY)		Oleoyl (OL)		Palmitoyl (PA)		Stearoyl (ST)	
C23	-0.0410	C23	-0.0400	C23	-0.0404	C23	-0.0408	C33	-0.0414
H3R	0.0150	H3R	0.0149	H3R	0.0147	H3R	0.0150	H3X	0.0152
H3S	0.0150	H3S	0.0149	H3S	0.0147	H3S	0.0150	H3Y	0.0152
C24	-0.0081	C24	-0.0086	C24	-0.0067	C24	-0.0084	C34	-0.0070
H4R	0.0084	H4R	0.0082	H4R	0.0083	H4R	0.0084	H4X	0.0081
H4S	0.0084	H4S	0.0082	H4S	0.0083	H4S	0.0084	H4Y	0.0081
C25	-0.0065	C25	-0.0054	C25	-0.0106	C25	-0.0063	C35	-0.0060
H5R	0.0062	H5R	0.0057	H5R	0.0065	H5R	0.0059	H5X	0.0056
H5S	0.0062	H5S	0.0057	H5S	0.0065	H5S	0.0059	H5Y	0.0056
C26	-0.0124	C26	-0.0109	C26	-0.0103	C26	-0.0105	C36	-0.0116
H6R	0.0045	H6R	0.0040	H6R	0.0055	H6R	0.0042	H6X	0.0040
H6S	0.0045	H6S	0.0040	H6S	0.0055	H6S	0.0042	H6Y	0.0040
C27	-0.0041	C27	-0.0078	C27	-0.0037	C27	-0.0077	C37	-0.0055
H7R	0.0032	H7R	0.0034	H7R	0.0077	H7R	0.0036	H7X	0.0034
H7S	0.0032	H7S	0.0034	H7S	0.0077	H7S	0.0036	H7Y	0.0034
C28	-0.0083	C28	-0.0061	C28	0.0466	C28	-0.0072	C38	-0.0074
H8R	0.0031	H8R	0.0040	H8R	0.0257	H8R	0.0039	H8X	0.0038
H8S	0.0031	H8S	0.0040	H8S	0.0257	H8S	0.0039	H8Y	0.0038
C29	-0.0132	C29	-0.0059	C29	-0.2343	C29	-0.0082	C39	-0.0093
H9R	0.0056	H9R	0.0036	H9R	0.1246	H9R	0.0038	H9X	0.0046
H9S	0.0056	H9S	0.0036	C210	-0.2357	H9S	0.0038	H9Y	0.0046
C210	-0.0066	C210	-0.0081	H10R	0.1247	C210	-0.0076	C310	-0.0071
H10R	0.0054	H10R	0.0031	C211	0.0447	H10R	0.0039	H10X	0.0038
H10S	0.0054	H10S	0.0031	H11R	0.0260	H10S	0.0039	H10Y	0.0038
C211	0.0294	C211	-0.0124	H11S	0.0260	C211	-0.0052	C311	-0.0105
H11R	-0.0013	H11R	0.0046	C212	-0.0043	H11R	0.0035	H11X	0.0044
H11S	-0.0013	H11S	0.0046	H12R	0.0084	H11S	0.0035	H11Y	0.0044
C212	-0.0684	C212	-0.0059	H12S	0.0084	C212	-0.0077	C312	-0.0091
H12R	0.0133	H12R	0.0054	C213	-0.0053	H12R	0.0032	H12X	0.0046
H12S	0.0133	H12S	0.0054	H13R	0.0047	H12S	0.0032	H12Y	0.0046
H12T	0.0133	C213	0.0303	H13S	0.0047	C213	-0.0127	C313	-0.0063
		H13R	-0.0016	C214	-0.0114	H13R	0.0044	H13X	0.0044
		H13S	-0.0016	H14R	0.0033	H13S	0.0044	H13Y	0.0044
		C214	-0.0688	H14S	0.0033	C214	-0.0059	C314	-0.0081
		H14R	0.0133	C215	-0.0103	H14R	0.0054	H14X	0.0037
		H14S	0.0133	H15R	0.0043	H14S	0.0054	H14Y	0.0037
		H14T	0.0133	H15S	0.0043	C215	0.0307	C315	-0.0147
				C216	-0.0039	H15R	-0.0014	H15X	0.0051
				H16R	0.0046	H15S	-0.0014	H15Y	0.0051
				H16S	0.0046	C216	-0.0706	C316	-0.0070
				C217	0.0316	H16R	0.0138	H16X	0.0055
				H17R	-0.0022	H16S	0.0138	H16Y	0.0055
				H17S	-0.0022	H16T	0.0138	C317	0.0319
				C218	-0.0684			H17X	-0.0015
				H18R	0.0130			H17Y	-0.0015
				H18S	0.0130			C318	-0.0714
				H18T	0.0130			H18X	0.0140
								H18Y	0.0140
								H18Z	0.0140

Table S3: Lennard–Jones parameters for the five atom types (C, O, OS, HC, and HA). The original AMBER parameters are in the upper row and Lipid14 parameters are in the lower row for each atom type.

Atom type	Radius (Å)	Well depth (kcal/mol)
C	1.9080	0.0860
Cox	1.9080	0.0700
O	1.6612	0.2100
Ox,OPx	1.6500	0.1400
OS	1.6837	0.1700
OSx,OTx	1.6500	0.1200
HC	1.4870	0.0157
HCx	1.4600	0.0100
HA	1.4590	0.0150
HAx	1.2500	0.0070

Table S4: Torsion dihedral parameters: n is the multiplicity, γ_n is the phase angle in degrees, and V_n is force constant in kilojoules per mol. The first column lists the four model molecules.

Model	Atom type	n	γ_n	V_n	Atom type	n	γ_n	V_n
(a)	CTx-CTx-CTx-CTx	1	180.0	0.0549	Cox-CTx-CTx-CTx	1	180.0	0.3965
		2	0.0	1.0368		2	0.0	0.9843
		3	0.0	1.3617		3	180.0	0.7506
		4	0.0	0.8602		4	0.0	0.4374
	OSx-Cox-CTx-CTx	1	180.0	0.8550	Ox-Cox-CTx-CTx	1	0.0	0.8550
		2	180.0	0.8843		2	180.0	0.8843
		3	180.0	0.0838		3	0.0	0.0838
		4	0.0	0.1152		4	0.0	0.1152
	C3-OSx-Cox-CTx	1	180.0	6.7006				
		2	180.0	10.8197				
		3	0.0	1.9895				
		4	180.0	0.7056				
(b)	CTx-C2-C2-CTx	1	180.0	6.8460	CTx-CTx-C2-C2	1	0.0	3.9021
		2	180.0	29.8084		2	180.0	2.4124
		3	0.0	0.8964		3	180.0	3.3800
		4	0.0	5.5361		4	180.0	1.4141
		5	180.0	2.1966				
		6	180.0	4.1360				
	CTx-CTx-CTx-C2	1	0.0	1.5160				
		2	0.0	2.3298				
		3	0.0	4.2690				
		4	180.0	0.8069				
(c)	OSx-C3-C3-OSx	1	180.0	2.1926	Cox-OSx-C3-C3	1	180.0	2.4789
		2	0.0	1.6375		2	180.0	3.6418
		3	180.0	1.5371		3	180.0	5.2369
		4	180.0	0.3040		4	180.0	0.7623
(d)	OTx-P5-OTx-C3	1	180.0	1.4765	P5-OTx-C3-C3	1	180.0	0.6004
		2	0.0	4.1542		2	0.0	0.5891
		3	0.0	0.7687		3	180.0	4.2784
		4	180.0	0.1103		4	0.0	1.0105
	OTx-C3-C3-N4x	1	180.0	6.4146				
		2	0.0	5.9014				
		3	0.0	4.1669				
		4	0.0	2.2285				

Table S5: RMSDs of the optimized structures in FUJI force field obtained from *ab initio* optimized structures (nm).

	(a)			
	CTx-CTx-CTx-CTx	Cox-CTx-CTx-CTx	OSx-Cox-CTx-CTx	C3-OSx-Cox-CTx
0	0.00008	0.00089	0.00033	0.00025
15	0.00166	0.00066	0.00035	0.00031
30	0.00040	0.00157	0.00043	0.00040
45	0.00179	0.00113	0.00053	0.00064
60	0.00227	0.00082	0.00057	0.00096
75	0.00091	0.00165	0.00060	0.00146
90	0.00050	0.00173	0.00071	0.00171
105	0.00034	0.00167	0.00041	0.00135
120	0.00012	0.00143	0.00035	0.00110
135	0.00009	0.00153	0.00036	0.00082
150	0.00012	0.00169	0.00034	0.00055
165	0.00009	0.00162	0.00031	0.00033
180	0.00003	0.00026	0.00026	0.00028

	(b)		
	CTx-CTx-C2-C2	CTx-CTx-CTx-C2	CTx-C2-C2-CTx
0	0.00627	0.08743	0.07285
15	0.00591	0.08341	0.05211
30	0.01017	0.09291	0.05276
45	0.02498	0.09441	0.05575
60	0.04097	0.09493	0.05876
75	0.05368	0.09529	0.06150
90	0.07403	0.09522	0.07015
105	0.07538	0.09315	0.08136
120	0.08061	0.09022	0.07297
135	0.06198	0.08636	0.06177
150	0.06113	0.08154	0.04991
165	0.06449	0.07809	0.03934
180	0.06927	0.07416	0.03521

	(c)		(d)		
	OSx-C3-C3-OSx	Cox-Osx-C3-C3	P5-OTx-C3-C3	OTx-P5-OTx-C3	Otx-C3-C3-N4x
0	0.02254	0.01070	0.00016	0.04136	0.05124
15	0.09076	0.01170	0.00019	0.04285	0.05123
30	0.05136	0.01363	0.00037	0.04362	0.05077
45	0.05765	0.07120	0.00035	0.04411	0.05082
60	0.05816	0.06009	0.00038	0.04464	0.05631
75	0.05124	0.05724	0.00026	0.01323	0.01921
90	0.03851	0.05293	0.00025	0.01362	0.05204
105	0.03572	0.04677	0.00035	0.05213	0.01131
120	0.04482	0.04151	0.00023	0.05017	0.00880
135	0.04032	0.03809	0.00018	0.01646	0.01026
150	0.03550	0.03602	0.00028	0.01045	0.02653
165	0.03376	0.03508	0.00031	0.00991	0.01145
180	0.03185	0.03408	0.00019	0.05897	0.08580

Table S6: Area per lipid for the seven lipid bilayers. The results of additional simulations ("additional runs" and "POPE (large)") and previous studies with the Lenard–Jones cutoff scheme (Refs. 10 and 11 for Lipid 14 and CHARRM36, respectively) are also presented.

Lipid	Temperature (K)	FUJI		Lipid14	CHARMM36	Experiment
		Primary runs	Additional runs			
DLPC	293	62.8 ± 0.1	62.6 ± 0.2			59.6[55]
	303	63.4 ± 0.2		63.0 ± 0.2	64.4 ± 0.3	60.8[55], 62.6[48], 63.2[51]
	323	65.1 ± 0.0				64.8[55], 67.1[48]
	333	66.0 ± 0.0				65.9[55]
	338					71.2[48]
DMPC	303	62.7 ± 0.1	62.4 ± 0.1	59.7 ± 0.7	60.8 ± 0.2	59.9[55], 60.0[48], 60.6[51], 60.6[52]
	323	64.3 ± 0.2				63.3[55], 65.4[48]
	333	65.9 ± 0.4				65.7[55]
	338					68.5[48]
DPPC	323	65.1 ± 0.2	65.1 ± 0.1	62.0 ± 0.3	62.9 ± 0.3	63.1[55], 63.3[48], 63.1[53],64.0[49]
	333	66.3 ± 0.1				65.0[55]
	338					67.1[48]
	353	68.5 ± 0.1				71.9[48]
DOPC	288	66.4 ± 0.3	67.1 ± 0.3			69.1[54]
	303	68.3 ± 0.1		69.0 ± 0.3	69.0 ± 0.3	72.4[54], 67.4[53], 72.4[52]
	318	69.4 ± 0.1				75.5[54]
POPC	293	65.5 ± 0.1	65.7 ± 0.1			62.7[55]
	303	66.6 ± 0.2		65.6 ± 0.5	64.7 ± 0.2	64.3[55], 68.3[52]
	323	68.3 ± 0.1				67.3[55]
	333	69.2 ± 0.1				68.1[55]
SOPC	293	64.8 ± 0.2	65.1 ± 0.2			63.8[55]
	303	66.3 ± 0.3				65.5[55]
	323	68.6 ± 0.1				68.1[55]
	333	69.6 ± 0.2				69.4[55]
POPE	293	58.0 ± 0.4	58.0 ± 0.2			
	303	58.6 ± 0.4				58.8[50]
	308					58.0[50], 59.7[50]
	310	59.2 ± 0.4		55.5 ± 0.2	59.2 ± 0.3	
	318					59.2[50], 61.7[50]
	323	60.7 ± 0.2				62.0[50]
	328					61.3[50]
	333	61.9 ± 0.2				63.3[50]
POPE (large)	293	Time step				
		5 fs	2 fs			
		56.8 ± 0.0	57.0 ± 0.0			

Table S7: Lateral diffusion coefficients of the seven lipid bilayers ($10^{-8} cm^2/s$).

	Temperature (K)	FUJI	Lipid14	CHARMM36	Experiment	References
DLPC	293	7.1 ± 0.1			8.5	Ref. 64
	298					
	303	12.2 ± 0.7	7.7			
	323	26.8 ± 1.3				
	333	34.9 ± 0.6				
DMPC	298				5.7	Ref. 66
	303	7.6 ± 0.3	5.1		6, 9	Ref. 63, Ref. 66
	313				9.2, 14.3	Ref. 63, Ref. 66
	319				11	Ref. 63
	323	17.1 ± 0.8			22.3	Ref. 66
	333	28.2 ± 1.9			13, 30.9	Ref. 67, Ref. 66
DPPC	319				12.1	Ref. 67
	323	14.7 ± 1.0	9.2	0.7 ± 0.1	12.3	Ref. 62
	324				15.2	Ref. 62
	328				13.7	Ref. 62
	333	20.9 ± 0.9				
	335				16.7	Ref. 62
	353	37.9 ± 0.2				
DOPC	283				3.1	Ref. 65
	288	4.1 ± 0.1				
	296				6.9	Ref. 65
	303	6.4 ± 0.2	6.5	7.8 ± 0.6	11.5	Ref. 66
	308				16	Ref. 68
	313				16	Ref. 66
	318	11.3 ± 0.9				
	323				22.2	Ref. 63
	333				29.3	Ref. 66
POPC	293	5.3 ± 0.3				
	303	8.6 ± 0.8	5.7	7.8 ± 0.9	10.7	Ref. 66
	313				15.3	Ref. 66
	323	15.9 ± 0.5			20.6	Ref. 66
	333	21.6 ± 0.6			28.3	Ref. 66
SOPC	293	4.3 ± 0.3				
	294				5	Ref. 68
	303	7.0 ± 0.5			7.7	Ref. 68
	313				12	Ref. 68
	323	16.0 ± 1.1			17	Ref. 68
	333	19.4 ± 1.5			24	Ref. 68
POPE	293	4.6 ± 0.6			3.4	Ref. 62
	303	6.7 ± 0.4			5	Ref. 62
	310	7.5 ± 0.9	4.7	6.0 ± 0.5		
	313				7.1	Ref. 62
	318				8.4	Ref. 62
	323	11.3 ± 0.8				
	333	21.4 ± 1.0				

Table S8: Lateral diffusion coefficients of the seven lipid bilayers from additional simulations for 200 ns and comparison with experiments. "Large" indicates a large system (6272 POPE lipids).

Lipid	Temperature (K)	Time step	Remarks	Diffusion coefficients ($10^{-8}cm^2/s$)	Experiments ($10^{-8}cm^2/s$)
DLPC	293	5 fs		8.1 ± 0.3	
DMPC	303	5 fs		7.6 ± 0.5	9[66]
DPPC	323	5 fs		14.7 ± 1.1	12.3[62]
DOPC	288	5 fs		4.1 ± 0.2	3.1[65]
POPC	293	5 fs		5.3 ± 0.2	
SOPC	294	5 fs		4.3 ± 0.2	5[68]
POPE	293	5 fs		4.6 ± 0.7	3.4[65]
		5 fs	large	4.0 ± 0.0	
		2 fs		3.6 ± 0.2	
		2 fs	large	3.9 ± 0.0	
		2 fs	no LJ-PME	4.2 ± 0.0	
		2 fs	no Vsite	4.7 ± 0.8	
		2 fs	no Vsite, no LJ-PME	4.7 ± 0.8	