Supporting Information:
Computing Individual Area per Head Group Reveals Lipid Bilayer Dynamics

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Table S1 provides examples of tessellation output, which indicate that the sum of all Delaunay (tetrahedra + polyhedra) equals the volume of the simulation box.

Table S2 provides averages and standard deviations for the Voronoi volume of each molecule type in each leaflet.

Table S3 provides details about degenerate polyhedra in simulations of the lipid system.

Table S4 indicates lipid contributions to regions of thickness 2.5 Å, rather than the 5 Å thickness employed in the main text.

Table S5 indicates the extent that lipid head group contributes to the overall average area that is occupied in each region by each lipid type.

Tables S6 and S7 list individual contributions from Na^+, Cl^-, and water to the area per lipid, when area is attributed solely to lipids.

Figure S1 and its accompanying text illustrate how the volume of a truncated tetrahedron was computed when it intersected planes that define the boundaries of a specified region.

Figure S2 shows the time decay of fluctuations in area and bilayer thickness.

Figure S3 shows the frequency of excursions out of the interface regions for all lipid types in both leaflets.

Figures S4 to S38 provide the area time autocorrelation of each lipid type in the inner and outer leaflets.

Table S1: Example of Voronoi Volume Comparison for Two Simulation Frames

659990 frame in dcd file
volume in tetrahedra only = 1502812.9125517488
volume omitted (tet in poly) 6.9532558196509337E-310
Nprimary= 155910
cutoff radius= 10.000000000000000 Å
ns= 425
nTetrahedra= 1085134 nTetDegenerate= 1
1502816.2652792530 $Å^3$ = expected volume
1502816.2652792733 $Å^3$ = total Delaunay volume (tetrahedra+polyhedra)
Epsi value = 1.0000000000000000E-008
660000 frame in dcd file
Nprimary= 155910
cutoff radius= 10.000000000000000
ns= 418
nTetrahedra= 1086335 nTetDegenerate= 0
1508635.1987842063 $Å^3$ = expected volume
1508635.1987842072 $Å^3$ = total Delaunay volume (tetrahedra+polyhedra)
Epsi value = 1.0000000000000000E-008

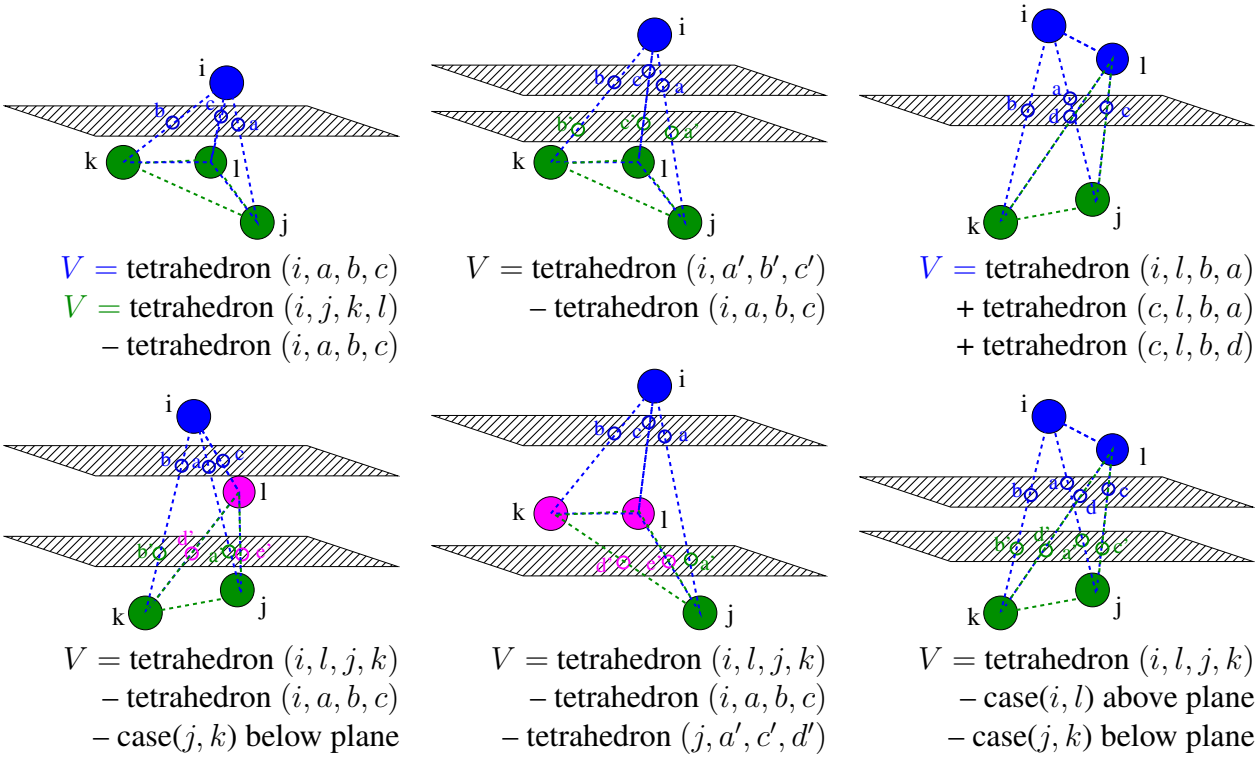

Figure S1: Full set of examples of how a tetrahedron can exist relative to two planes that define boundaries of a planar region. Equations illustrate how the volume that remains in the region is computed.

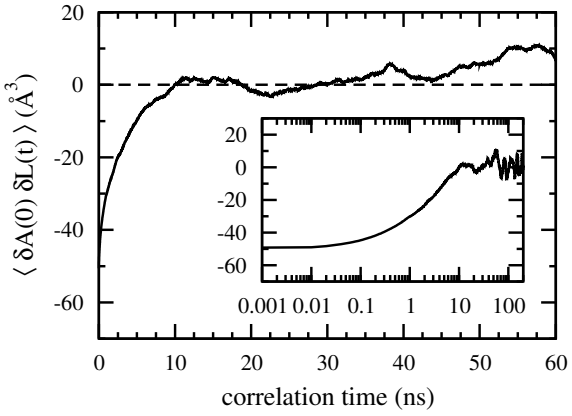

Figure S2: Coupled fluctuations in area and distance between average P atom locations, relative to average area $\langle A \rangle$ and average length $\langle L \rangle$, at a time separation t. The logarithmic time scale (inset) emphasizes the decay at early times.

Table S2: Average Voronoi Molecule Volume and Head Group Volume Per Molecule Type

	inner leaflet				outer leaflet			
molecule	V (Å^3)	std dev	head V	std dev	V (Å^3)	std dev	head V	std dev
PG (a15:0/a15:0)	1122.77	33.52	289.05	10.62	1124.53	33.36	289.42	10.74
PG (i15:0/a15:0)	1123.38	33.29	289.10	10.60	1124.68	33.52	289.33	10.70
PG (16:0/a15:0)	1152.55	33.87	289.00	10.54	1154.39	34.29	289.12	10.70
PG (a17:0/a15:0)	1179.67	34.28	289.01	10.59	1181.11	34.44	289.15	10.68
PG (i17:0/a15:0)	1181.04	33.79	289.12	10.57	1182.59	34.50	289.35	10.74
PG (a17:0/i15:0)	1181.09	34.48	289.16	10.60	1183.84	34.55	289.50	10.76
PG (i17:0/i15:0)	1181.65	34.57	289.16	10.63	1184.60	34.37	289.39	10.70
PG (18:0/a15:0)	1211.10	34.97	289.31	10.69	1212.35	35.10	289.17	10.70
PG (18:1/a15:0)	1200.19	34.57	289.62	10.76	1200.79	34.69	289.18	10.67
PG (18:1/i15:0)	1200.17	34.71	288.94	10.54	1202.34	34.72	289.28	10.72
PG (a19:0/a15:0)	1237.18	35.22	289.00	10.59	1238.69	35.20	289.20	10.72
PG (i19:0/a15:0)	1238.94	35.14	289.16	10.64	1240.03	35.28	289.22	10.67
PG (a19:0/i15:0)	1237.66	35.39	288.74	10.57	1238.85	35.29	289.08	10.67
PG (20:0/a15:0)	1268.30	35.46	289.12	10.65	1268.65	35.51	288.93	10.59
CL (a17:0/a15:0)	2226.42	51.59	445.47	12.75	2228.14	51.69	445.57	12.85
LPG (a17:0/a15:0)	1385.64	36.36	493.72	14.56	1388.63	36.55	494.78	14.94
LPG (i17:0/a15:0)	1386.72	36.23	493.95	14.63				
LPG (18:0/a15:0)	1416.75	36.70	493.89	14.51				
LPG (a19:0/a15:0)	1442.46	37.11	493.77	14.54				
Na^+	5238.79	23.17	(in entire box)					
Cl^-	1115.22	12.50	(in entire box)					
H_2O	1012618.48	1383.31	(in entire box)					

Table S3: Details about Delaunay Degenerate Polyhedra in Membrane Simulations

60,000	simulation time steps analyzed (1 per 10 ps)
65,139,407,177	total number of tetrahedra
51,704	# of time steps with 0 degenerate polyhedra
7699	# of time steps with 1 degenerate polyhedra
565	# of time steps with 2 degenerate polyhedra
32	# of time steps with 3 degenerate polyhedra
8296	total # time steps with degenerate polyhedra
8925	degenerate polyhedra with 5 vertices
0	degenerate polyhedra with 6 or more vertices
0	cases with vertices being only ions
6250	cases with vertices being only atoms in water
1750	cases with vertices being only atoms in lipids
113	cases with vertices being water and ion(s)
1	cases with vertices being lipids and ion(s)
790	cases with vertices being water and lipid(s)
21	cases with vertices being water, lipid(s), and ion(s)

Table S4: Lipid Contributions to Area within Each 2.5 Å Region

	water side, 5 to 2.5 Å				2.5 to 0 Å			
lipid and	inner leaflet		outer leaflet		inner leaflet		outer leaflet	
contributions (Å^2)	area	std dev	area	std dev	area	std dev	area	std dev
PG (a15:0/a15:0)	14.08	15.12	13.07	14.94	25.30	17.36	24.67	17.96
PG (i15:0/a15:0)	15.76	15.58	13.28	14.96	27.59	17.65	25.02	17.81
PG (16:0/a15:0)	15.59	15.87	13.89	15.22	26.83	17.98	25.21	18.07
PG (a17:0/a15:0)	13.31	15.24	13.49	15.14	24.29	17.94	24.95	18.03
PG (i17:0/a15:0)	14.58	15.75	13.05	15.00	26.07	18.33	24.44	17.94
PG (a17:0/i15:0)	15.11	15.58	11.61	14.32	26.64	17.56	21.81	17.46
PG (i17:0/i15:0)	15.05	15.92	12.32	14.87	26.20	17.83	23.37	18.43
PG (18:0/a15:0)	13.83	15.93	13.16	14.97	25.00	18.92	24.75	18.04
PG (18:1/a15:0)	13.04	15.33	13.27	15.15	23.70	18.49	24.00	18.27
PG (18:1/i15:0)	16.01	15.82	13.04	15.19	27.49	17.83	24.06	18.34
PG (a19:0/a15:0)	15.70	15.87	12.47	14.58	27.59	17.90	23.90	17.75
PG (i19:0/a15:0)	15.35	15.85	13.74	15.19	27.23	18.04	25.35	18.05
PG (a19:0/i15:0)	16.27	15.91	14.26	15.35	27.49	17.83	25.95	17.93
PG (20:0/a15:0)	14.14	15.43	14.18	15.39	25.49	18.24	25.62	18.15
CL (a17:0/a15:0)	15.63	20.94	16.14	21.01	37.21	28.67	38.54	28.79
LPG (a17:0/a15:0)	20.52	24.16	14.71	22.59	36.54	27.97	29.65	29.34
LPG (i17:0/a15:0)	23.08	25.20			39.46	28.26		
LPG (18:0/a15:0)	21.82	25.05			37.61	28.48		
LPG (a19:0/a15:0)	25.12	25.88			41.76	28.01		
	membrane side, 0 to 2.5 Å				2.5 to 5 Å			
	inner leaflet		outer leaflet		inner leaflet		outer leaflet	
PG (a15:0/a15:0)	37.93	18.05	38.47	19.20	50.08	18.17	51.63	18.88
PG (i15:0/a15:0)	40.41	18.35	38.19	18.70	52.35	18.53	50.75	18.34
PG (16:0/a15:0)	39.15	18.38	38.31	19.33	50.50	17.96	51.17	19.28
PG (a17:0/a15:0)	37.21	18.62	38.12	18.71	49.71	18.07	50.76	18.32
PG (i17:0/a15:0)	39.12	18.83	37.74	19.01	51.61	18.57	50.82	18.82
PG (a17:0/i15:0)	38.83	17.86	34.03	18.54	50.27	17.32	46.94	18.12
PG (i17:0/i15:0)	38.45	18.10	36.30	19.60	50.13	18.10	49.57	19.30
PG (18:0/a15:0)	37.55	19.42	38.03	19.04	49.54	18.44	50.37	18.39
PG (18:1/a15:0)	36.43	19.75	37.10	20.02	50.04	20.21	51.17	20.43
PG (18:1/i15:0)	39.81	18.70	37.62	19.92	52.44	19.52	52.26	20.56
PG (a19:0/a15:0)	40.15	17.95	37.25	18.93	51.49	17.17	50.52	18.79
PG (i19:0/a15:0)	39.70	18.24	38.68	18.92	51.58	18.21	51.46	18.60
PG (a19:0/i15:0)	39.49	18.15	38.93	18.48	50.96	17.81	51.13	17.81
PG (20:0/a15:0)	38.21	19.11	38.32	19.34	50.80	18.77	50.83	19.07
CL (a17:0/a15:0)	64.70	30.66	66.52	31.00	91.95	29.05	94.36	29.64
LPG (a17:0/a15:0)	52.49	27.13	49.03	31.34	63.37	24.74	66.62	28.72
LPG (i17:0/a15:0)	55.04	27.39			65.41	25.10		
LPG (18:0/a15:0)	53.28	27.20			64.71	24.57		
LPG (a19:0/a15:0)	56.32	26.70			64.37	24.40		

Table S5: Fraction of Lipid Area Contribution Made by Head Group

lipid	fraction, water side				fraction, membrane side			
	5 to 2.5 Å		2.5 to 0 Å		0 to 2.5 Å		2.5 to 5 Å	
	inner	outer	inner	outer	inner	outer	inner	outer
PG (a15:0/a15:0)	0.971	0.966	0.896	0.894	0.726	0.730	0.471	0.479
PG (i15:0/a15:0)	0.963	0.973	0.876	0.900	0.688	0.734	0.424	0.480
PG (16:0/a15:0)	0.960	0.970	0.869	0.892	0.686	0.713	0.439	0.464
PG (a17:0/a15:0)	0.966	0.971	0.890	0.896	0.728	0.728	0.490	0.479
PG (i17:0/a15:0)	0.958	0.970	0.870	0.896	0.693	0.731	0.447	0.484
PG (a17:0/i15:0)	0.967	0.978	0.882	0.915	0.700	0.768	0.450	0.537
PG (i17:0/i15:0)	0.958	0.973	0.870	0.901	0.698	0.739	0.454	0.502
PG (18:0/a15:0)	0.955	0.971	0.867	0.898	0.699	0.732	0.472	0.484
PG (18:1/a15:0)	0.959	0.970	0.879	0.892	0.714	0.713	0.478	0.467
PG (18:1/i15:0)	0.961	0.962	0.875	0.886	0.684	0.718	0.420	0.473
PG (a19:0/a15:0)	0.958	0.976	0.873	0.908	0.689	0.746	0.432	0.497
PG (i19:0/a15:0)	0.961	0.974	0.878	0.898	0.695	0.721	0.437	0.465
PG (a19:0/i15:0)	0.956	0.967	0.865	0.890	0.673	0.716	0.419	0.462
PG (20:0/a15:0)	0.962	0.965	0.880	0.883	0.709	0.706	0.465	0.459
CL (a17:0/a15:0)	0.957	0.959	0.882	0.881	0.715	0.707	0.463	0.448
LPG (a17:0/a15:0)	0.987	0.984	0.950	0.945	0.851	0.856	0.661	0.697
LPG (i17:0/a15:0)	0.985		0.940		0.822		0.607	
LPG (18:0/a15:0)	0.984		0.943		0.839		0.643	
LPG (a19:0/a15:0)	0.977		0.919		0.793		0.578	

Table S6: Contribution of each Molecule Type to Area Per Head Group in Outer Leaflet

		Area (Å^2) arising from				
Lipid name	number	lipid	Na^+	Cl^-	H_2O	total
Outer leaflet, P to water						
PG (a15:0/a15:0)	9	18.86729	0.86096	0.00487	49.96486	69.69798
PG (i15:0/a15:0)	7	19.14873	0.87380	0.00494	50.71017	70.73765
PG (16:0/a15:0)	8	19.54916	0.89208	0.00505	51.77059	72.21687
PG (a17:0/a15:0)	34	19.21883	0.87700	0.00496	50.89581	70.99661
PG (i17:0/a15:0)	21	18.74664	0.85545	0.00484	49.64533	69.25226
PG (a17:0/i15:0)	4	16.70799	0.76243	0.00431	44.24654	61.72127
PG (i17:0/i15:0)	5	17.84342	0.81424	0.00461	47.25341	65.91567
PG (18:0/a15:0)	19	18.95672	0.86504	0.00489	50.20169	70.02835
PG (18:1/a15:0)	4	18.63371	0.85030	0.00481	49.34627	68.83509
PG (18:1/i15:0)	5	18.54967	0.84647	0.00479	49.12373	68.52466
PG (a19:0/a15:0)	11	18.18362	0.82976	0.00469	48.15434	67.17242
PG (i19:0/a15:0)	12	19.54905	0.89207	0.00505	51.77031	72.21648
PG (a19:0/i15:0)	12	20.10220	0.91731	0.00519	53.23518	74.25989
PG (20:0/a15:0)	11	19.89869	0.90803	0.00514	52.69624	73.50810
CL (a17:0/a15:0)	15	27.34314	1.24773	0.00706	72.41083	101.00876
LPG (a17:0/a15:0)	8	22.17978	1.01212	0.00573	58.73707	81.93470

		Area (Å^2) arising from				
Lipid name	number	lipid	Na^+	Cl^-	H_2O	total
Outer leaflet, P to membrane						
PG (a15:0/a15:0)	9	45.050345	0.645964	0.000315	23.314673	69.011297
PG (i15:0/a15:0)	7	44.468730	0.637624	0.000311	23.013672	68.120338
PG (16:0/a15:0)	8	44.742861	0.641555	0.000313	23.155542	68.540271
PG (a17:0/a15:0)	34	44.440576	0.637221	0.000311	22.999102	68.077209
PG (i17:0/a15:0)	21	44.279345	0.634909	0.000310	22.915661	67.830225
PG (a17:0/i15:0)	4	40.481144	0.580447	0.000283	20.949998	62.011873
PG (i17:0/i15:0)	5	42.933556	0.615612	0.000301	22.219182	65.768650
PG (18:0/a15:0)	19	44.203803	0.633826	0.000309	22.876566	67.714504
PG (18:1/a15:0)	4	44.136934	0.632867	0.000309	22.841960	67.612070
PG (18:1/i15:0)	5	44.939600	0.644376	0.000315	23.257359	68.841649
PG (a19:0/a15:0)	11	43.886991	0.629283	0.000307	22.712608	67.229189
PG (i19:0/a15:0)	12	45.068724	0.646227	0.000315	23.324184	69.039450
PG (a19:0/i15:0)	12	45.029638	0.645667	0.000315	23.303956	68.979576
PG (20:0/a15:0)	11	44.574607	0.639142	0.000312	23.068466	68.282527
CL (a17:0/a15:0)	15	80.439651	1.153401	0.000563	41.629517	123.223133
LPG (a17:0/a15:0)	8	57.822463	0.829100	0.000405	29.924560	88.576527

Table S7: Contribution of each Molecule Type to Area Per Head Group in Inner Leaflet

		Area (Å^2) arising from				
Lipid name	number	lipid	Na^+	Cl^-	H_2O	total
Inner leaflet, P to membrane						
PG (a15:0/a15:0)	9	44.006138	0.265358	0.000447	17.965896	62.237839
PG (i15:0/a15:0)	7	46.378626	0.279664	0.000471	18.934486	65.593247
PG (16:0/a15:0)	8	44.823609	0.270287	0.000455	18.299636	63.393988
PG (a17:0/a15:0)	11	43.462502	0.262079	0.000441	17.743952	61.468975
PG (i17:0/a15:0)	4	45.364027	0.273546	0.000461	18.520267	64.158300
PG (a17:0/i15:0)	9	44.552560	0.268652	0.000453	18.188978	63.010643
PG (i17:0/i15:0)	4	44.290193	0.267070	0.000450	18.081864	62.639577
PG (18:0/a15:0)	10	43.544953	0.262577	0.000442	17.777613	61.585585
PG (18:1/a15:0)	5	43.235154	0.260709	0.000439	17.651135	61.147436
PG (18:1/i15:0)	4	46.125326	0.278136	0.000469	18.831074	65.235005
PG (a19:0/a15:0)	10	45.821268	0.276303	0.000465	18.706939	64.804976
PG (i19:0/a15:0)	12	45.639131	0.275205	0.000464	18.632580	64.547380
PG (a19:0/i15:0)	9	45.226378	0.272716	0.000459	18.464070	63.963624
PG (20:0/a15:0)	11	44.500644	0.268339	0.000452	18.167783	62.937218
CL (a17:0/a15:0)	15	78.326350	0.472309	0.000796	31.977428	110.776882
LPG (a17:0/a15:0)	26	57.929722	0.349317	0.000588	23.650323	81.929950
LPG (i17:0/a15:0)	18	60.225089	0.363158	0.000612	24.587427	85.176287
LPG (18:0/a15:0)	9	58.991603	0.355720	0.000599	24.083846	83.431768
LPG (a19:0/a15:0)	4	60.344599	0.363879	0.000613	24.636218	85.345308

		Area (Å^2) arising from				
Lipid name	number	lipid	Na^+	Cl^-	H_2O	total
Inner leaflet, P to water						
PG (a15:0/a15:0)	9	19.68608	0.44055	0.00625	40.31616	60.44904
PG (i15:0/a15:0)	7	21.67658	0.48510	0.00688	44.39259	66.56114
PG (16:0/a15:0)	8	21.21163	0.47469	0.00673	43.44041	65.13346
PG (a17:0/a15:0)	11	18.79839	0.42069	0.00597	38.49820	57.72324
PG (i17:0/a15:0)	4	20.32869	0.45493	0.00645	41.63219	62.42227
PG (a17:0/i15:0)	9	20.87193	0.46709	0.00662	42.74472	64.09036
PG (i17:0/i15:0)	4	20.62522	0.46157	0.00654	42.23947	63.33280
PG (18:0/a15:0)	10	19.41491	0.43448	0.00616	39.76081	59.61637
PG (18:1/a15:0)	5	18.36953	0.41109	0.00583	37.61992	56.40636
PG (18:1/i15:0)	4	21.74876	0.48671	0.00690	44.54041	66.78278
PG (a19:0/a15:0)	10	21.64378	0.48436	0.00687	44.32543	66.46045
PG (i19:0/a15:0)	12	21.29044	0.47645	0.00676	43.60180	65.37544
PG (a19:0/i15:0)	9	21.87886	0.48962	0.00694	44.80687	67.18230
PG (20:0/a15:0)	11	19.81636	0.44347	0.00629	40.58295	60.84906
CL (a17:0/a15:0)	15	26.41951	0.59124	0.00838	54.10590	81.12503
LPG (a17:0/a15:0)	26	28.52971	0.63846	0.00905	58.42748	87.60470
LPG (i17:0/a15:0)	18	31.27075	0.69980	0.00992	64.04100	96.02148
LPG (18:0/a15:0)	9	29.71385	0.66496	0.00943	60.85255	91.24079
LPG (a19:0/a15:0)	4	33.44117	0.74837	0.01061	68.48591	102.68606

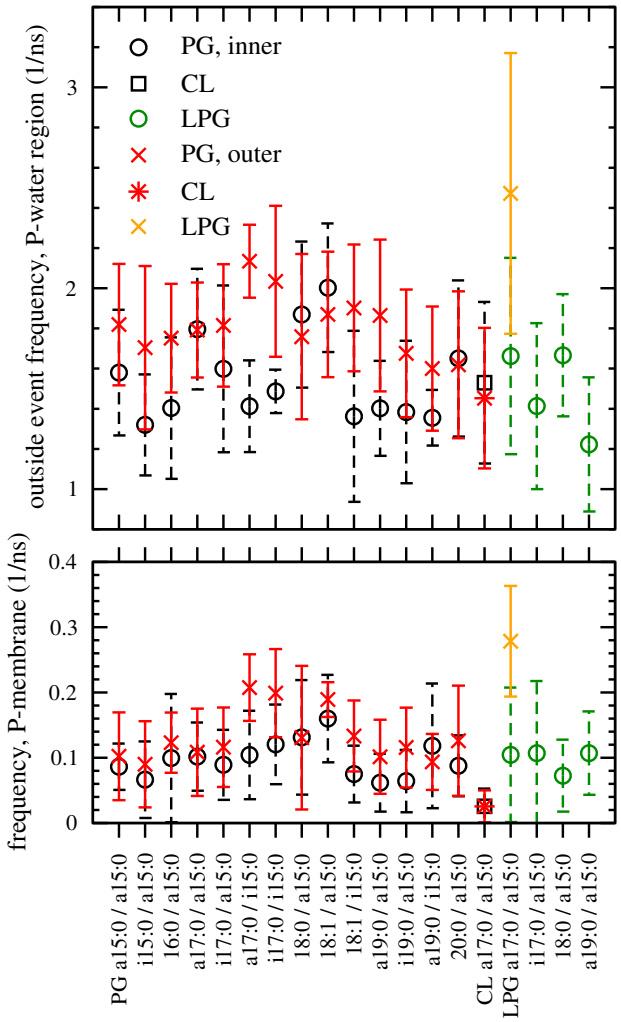

Figure S3: Frequency of excursions that led to zero contribution to the Voronoi volume that extend 5 Å from a plane of average P positions (a) toward the bulk water phase and (b) into the bilayer. Symbols and colors distinguish lipids and leaflets, as in figures in the main text.

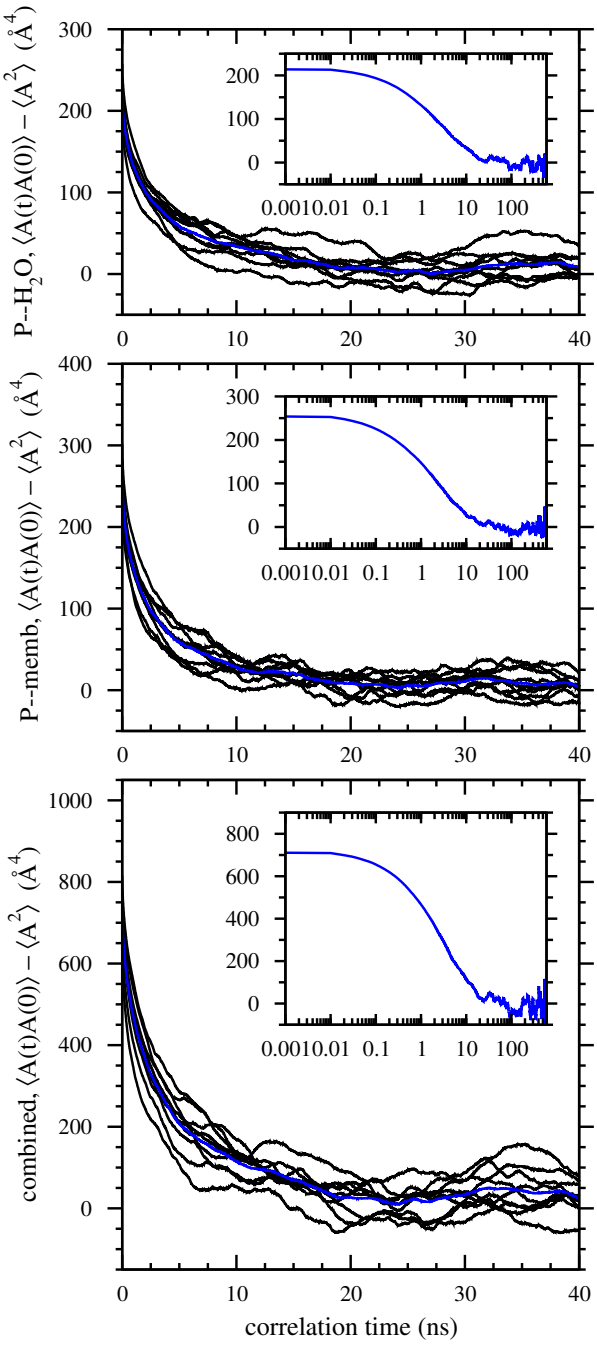

Figure S4: Relaxation of the contributions made by PG(a15:0/a15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the inner leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

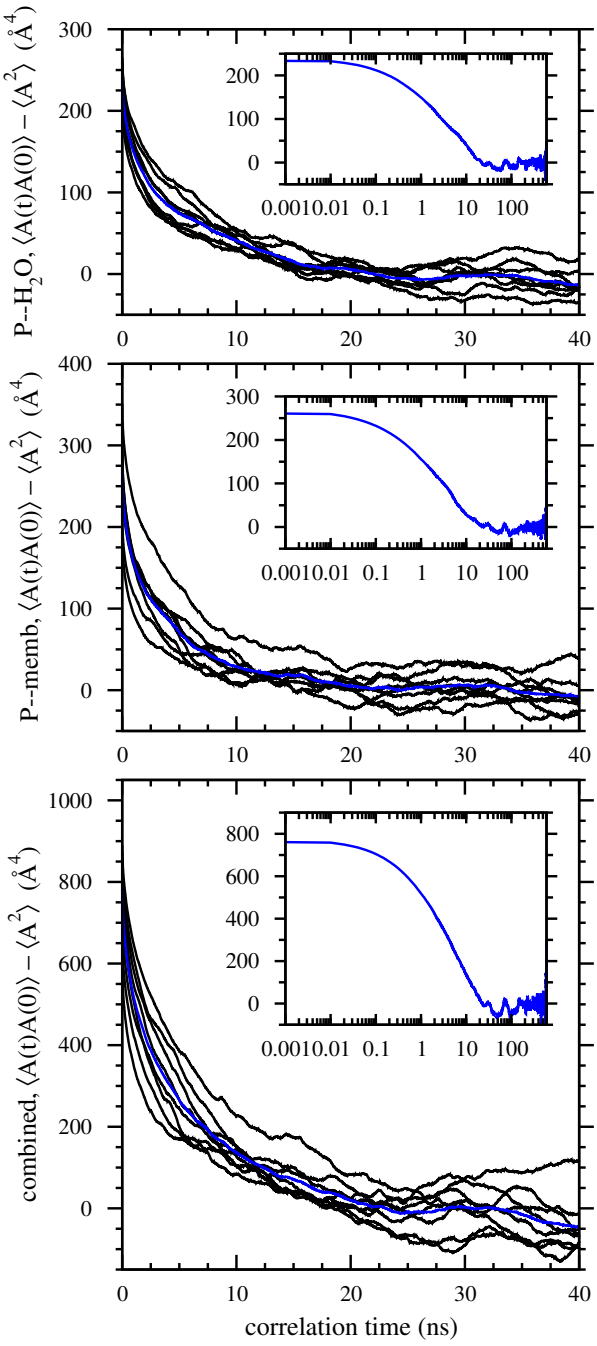

Figure S5: Relaxation of the contributions made by PG(i15:0/a15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the inner leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

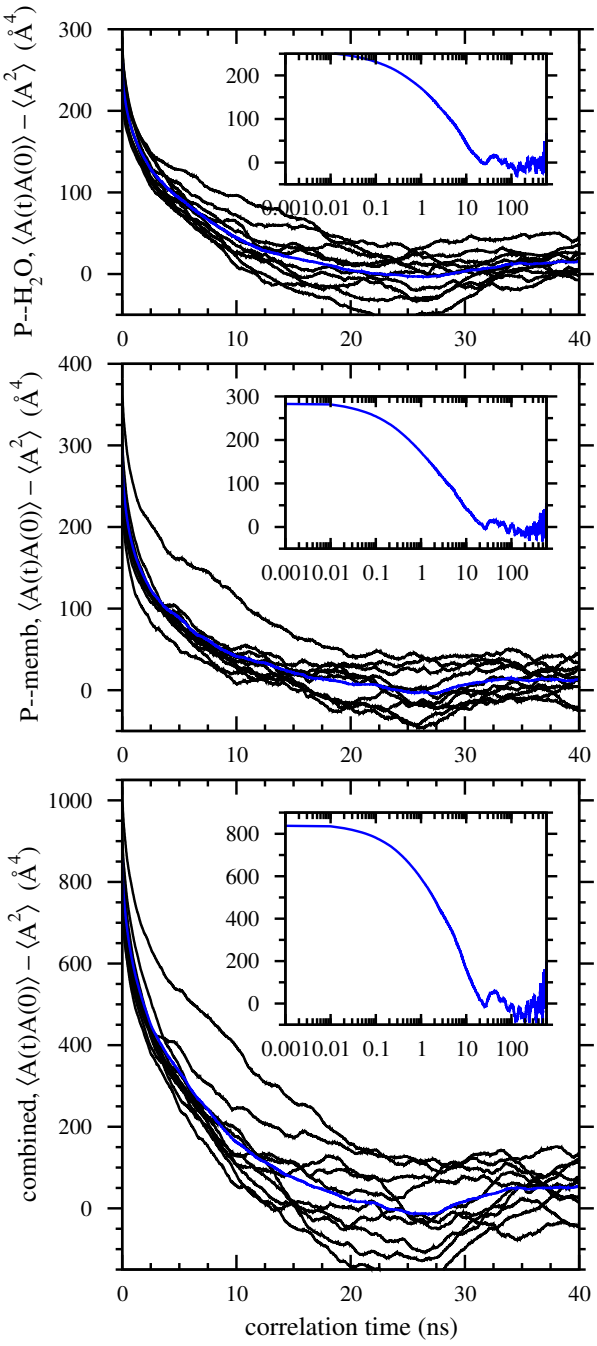

Figure S6: Relaxation of the contributions made by PG(16:0/a15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the inner leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

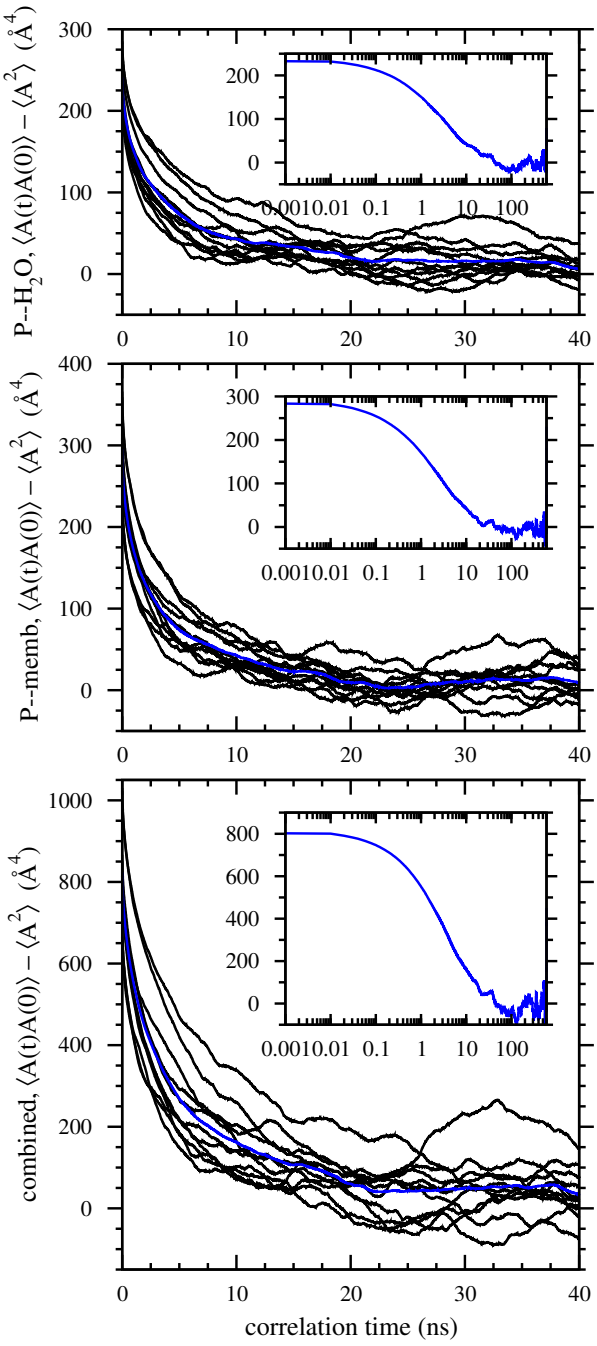

Figure S7: Relaxation of the contributions made by PG(a17:0/a15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the inner leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

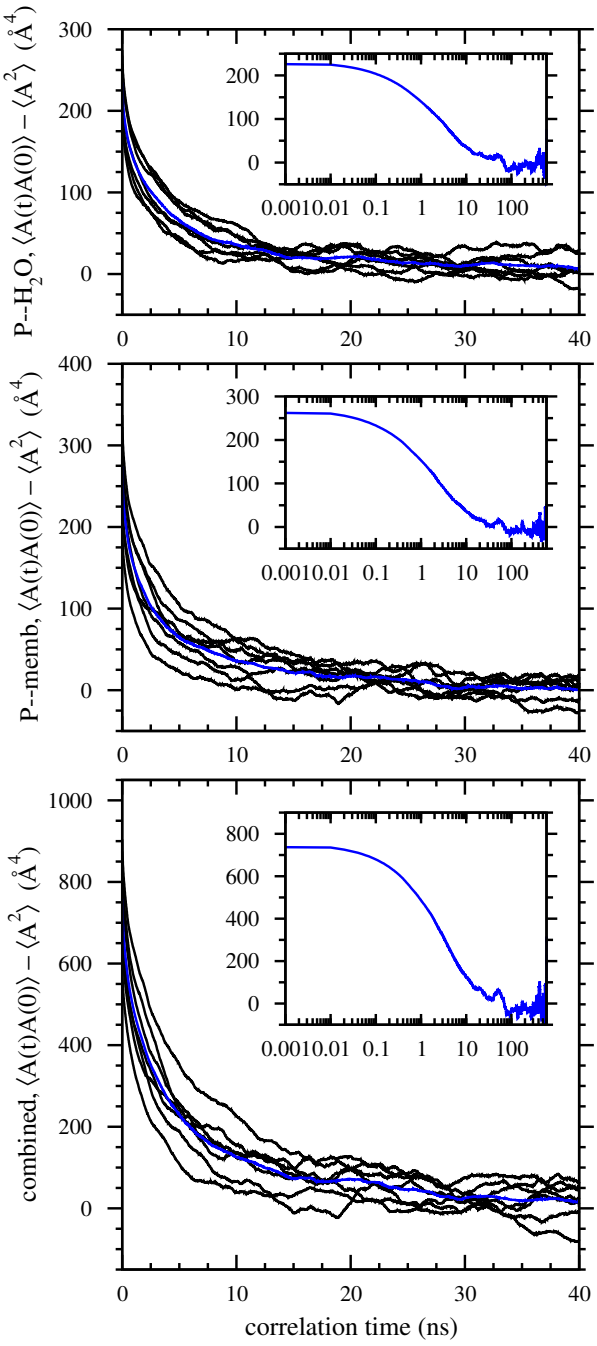

Figure S8: Relaxation of the contributions made by PG(i17:0/a15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the inner leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

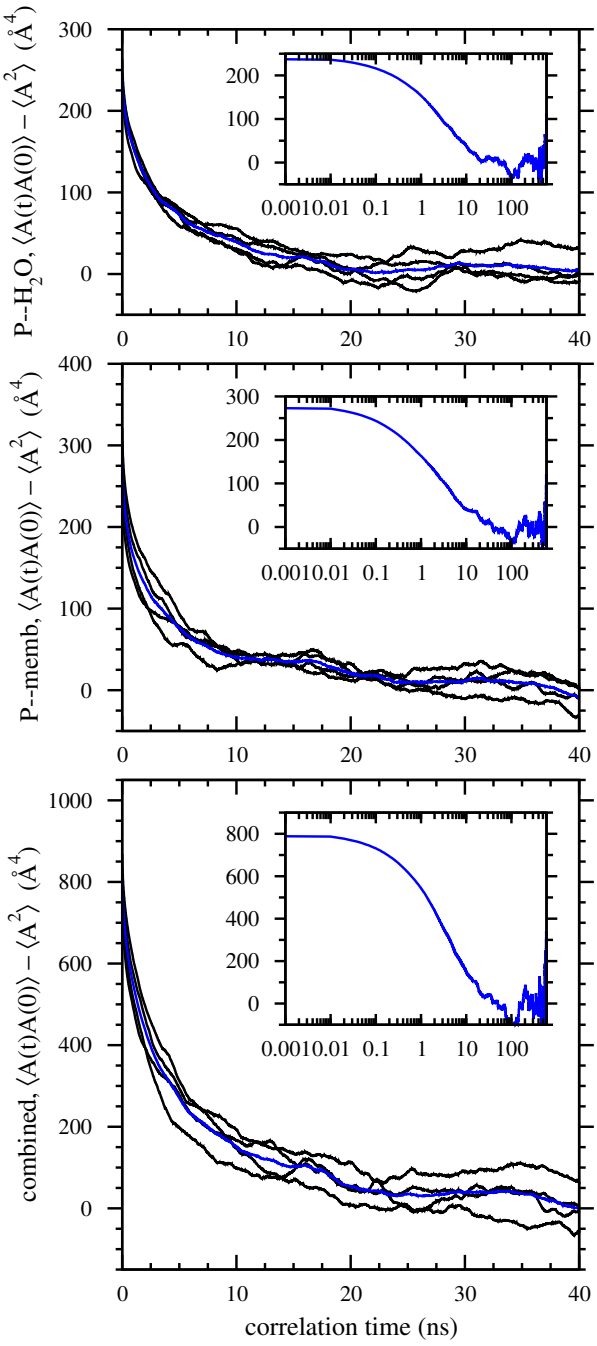

Figure S9: Relaxation of the contributions made by PG(a17:0/i15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the inner leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

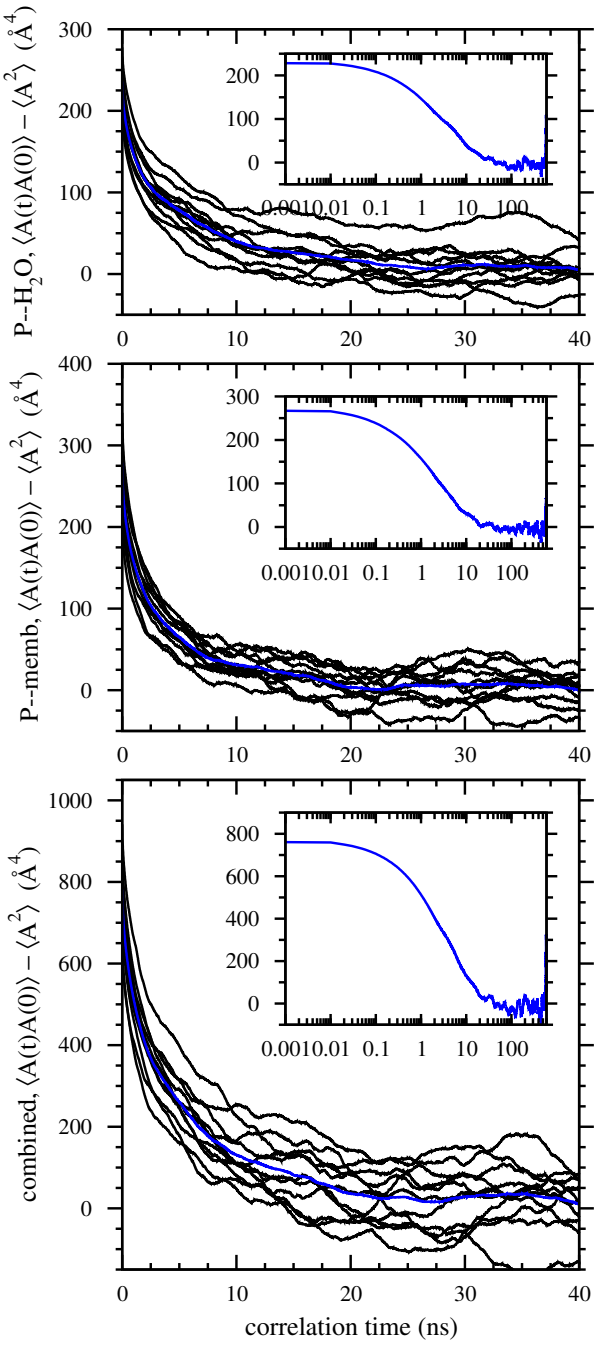

Figure S10: Relaxation of the contributions made by PG(i17:0/i15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the inner leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

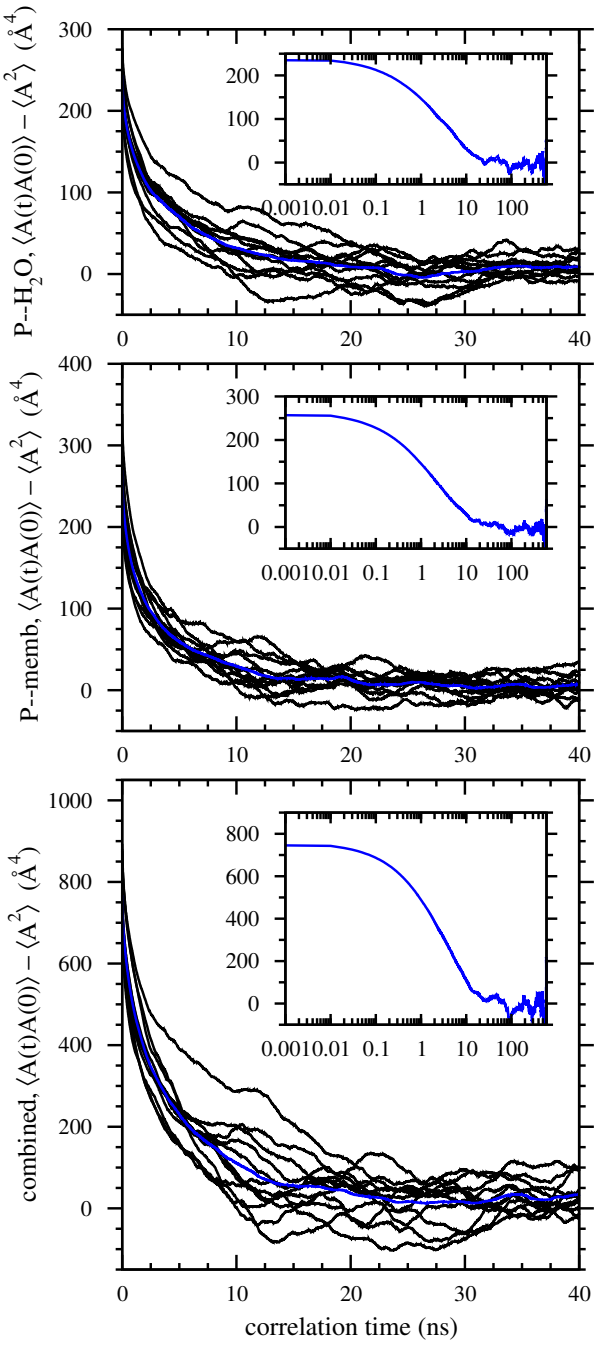

Figure S11: Relaxation of the contributions made by PG(18:0/a15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the inner leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

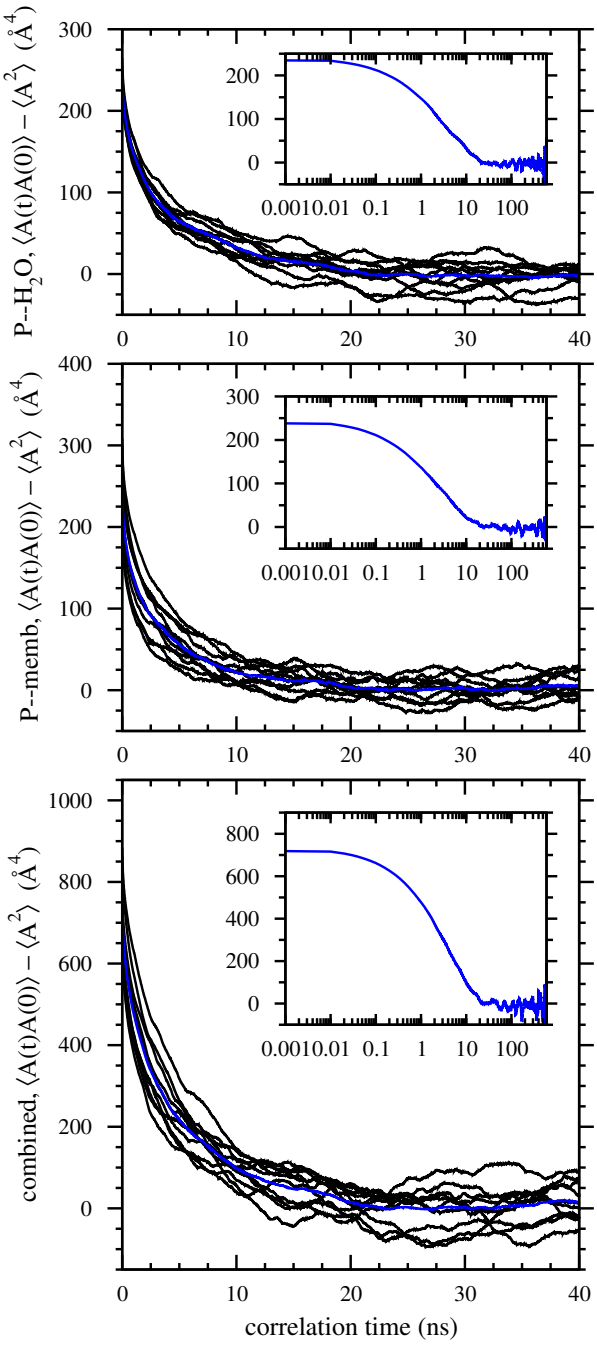

Figure S12: Relaxation of the contributions made by PG(18:1/a15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the inner leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

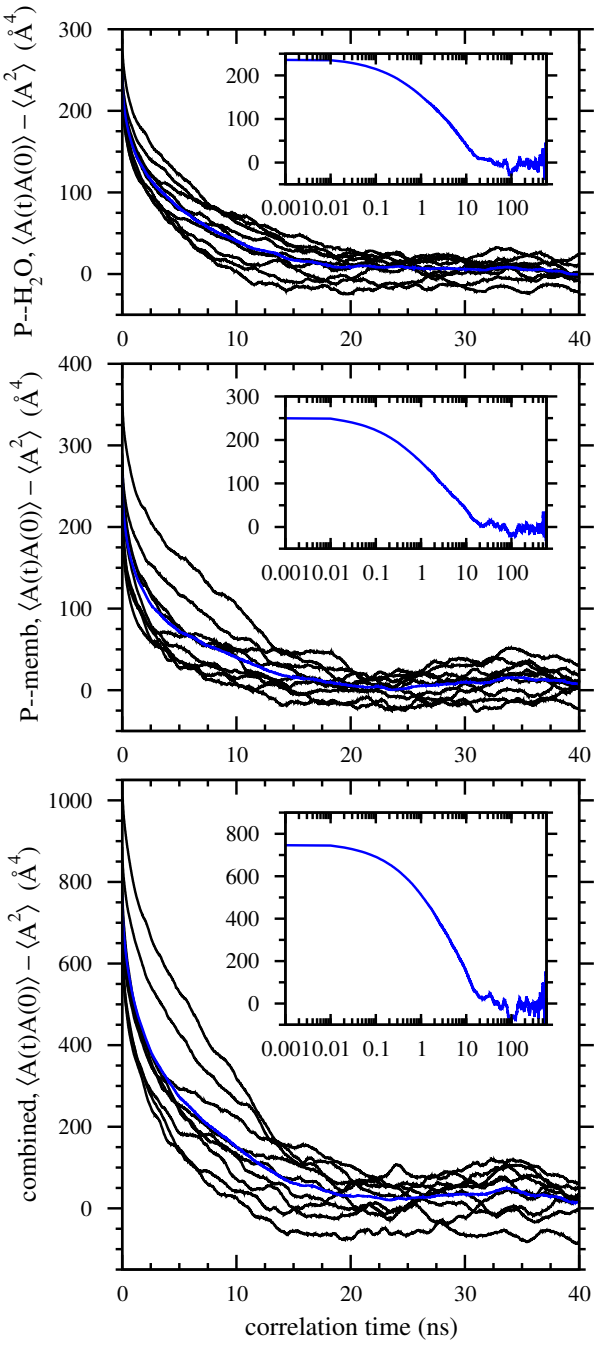

Figure S13: Relaxation of the contributions made by PG(18:1/i15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the inner leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

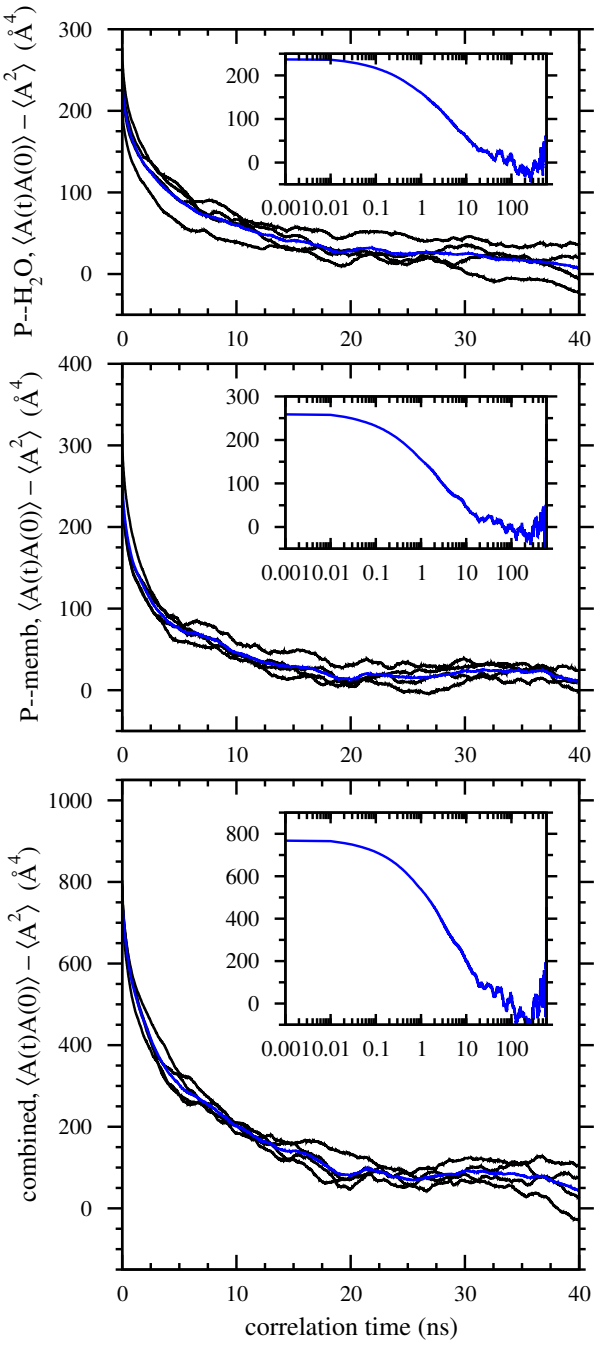

Figure S14: Relaxation of the contributions made by PG(a19:0/a15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the inner leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

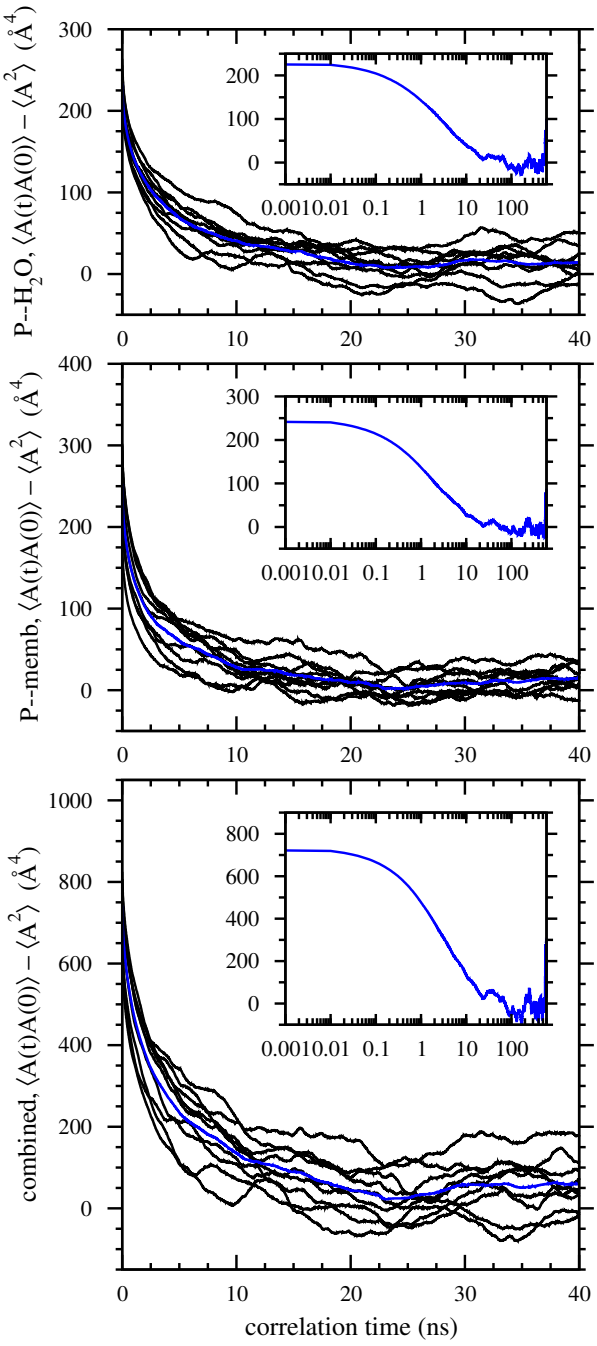

Figure S15: Relaxation of the contributions made by PG(i19:0/a15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the inner leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

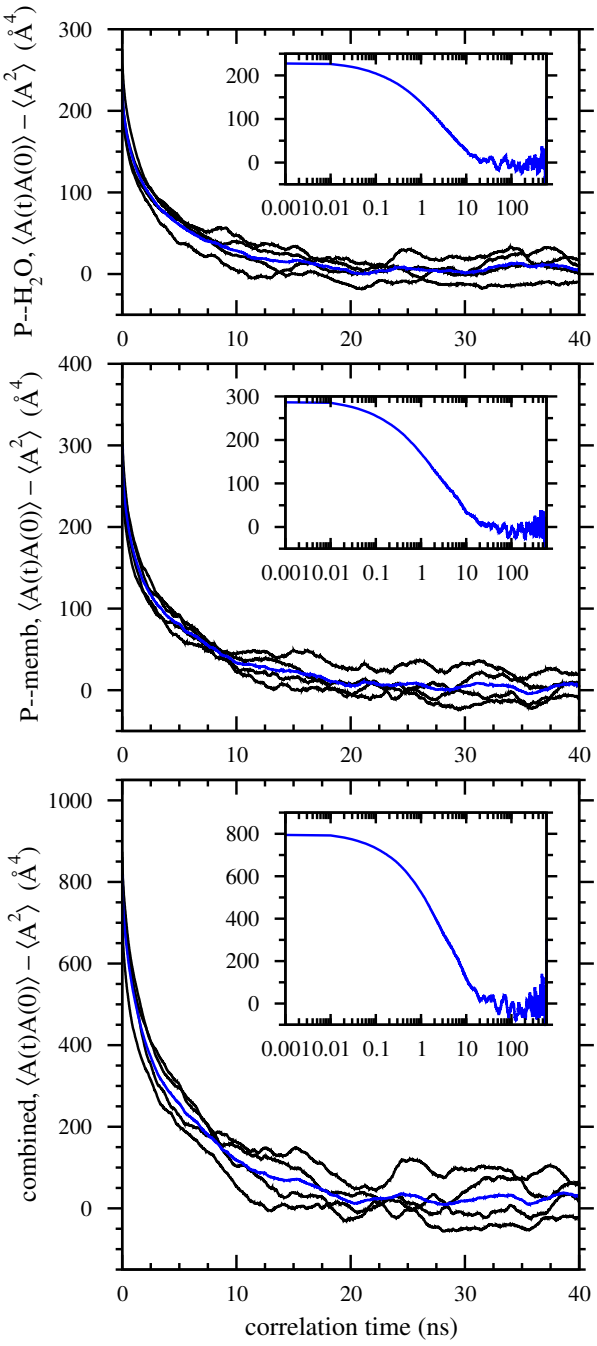

Figure S16: Relaxation of the contributions made by PG(a19:0/i15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the inner leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

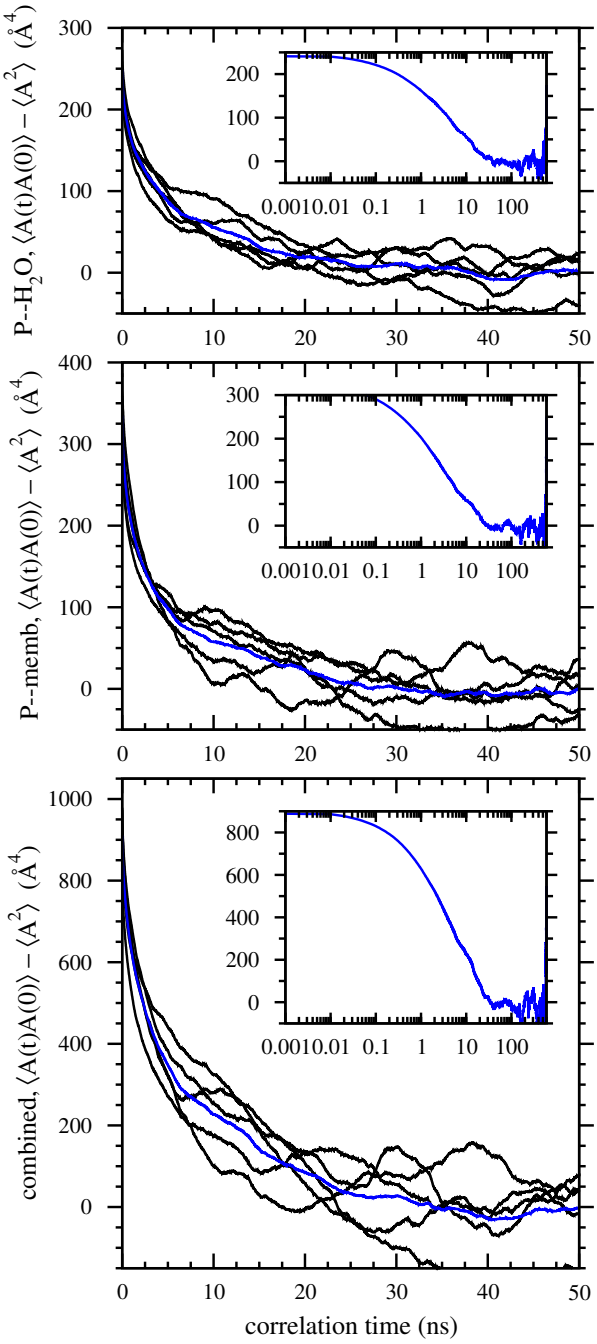

Figure S17: Relaxation of the contributions made by PG(20:0/a15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the inner leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

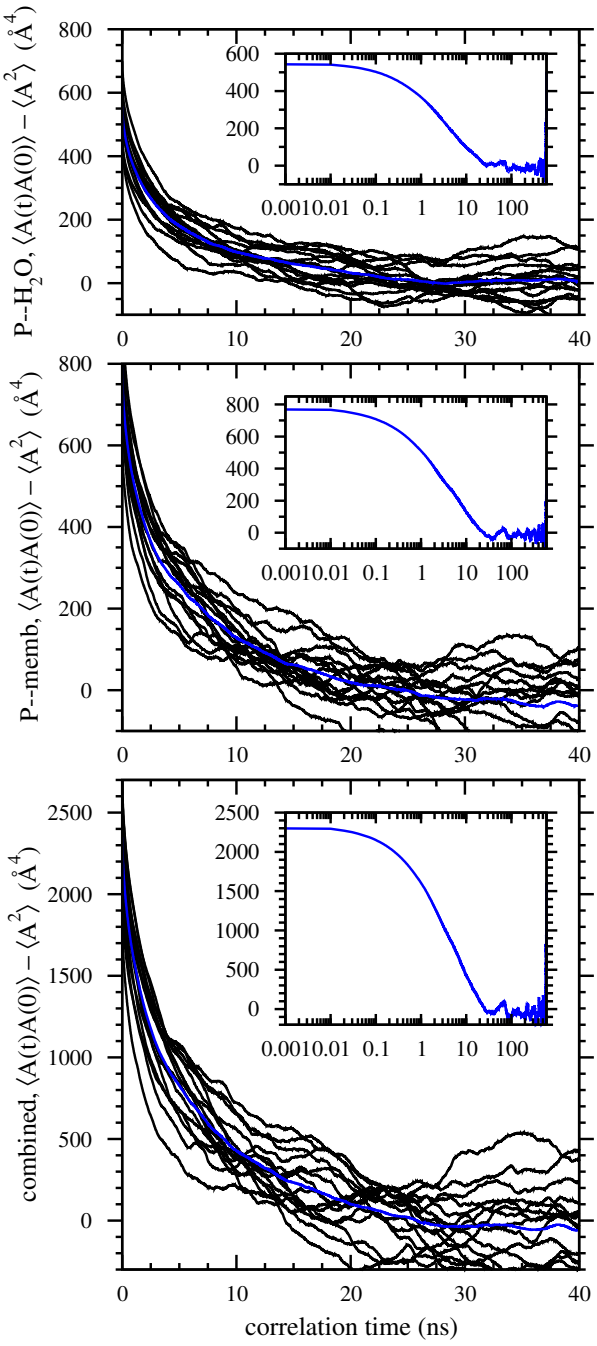

Figure S18: Relaxation of the contributions made by PG(a17:0/a15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the inner leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

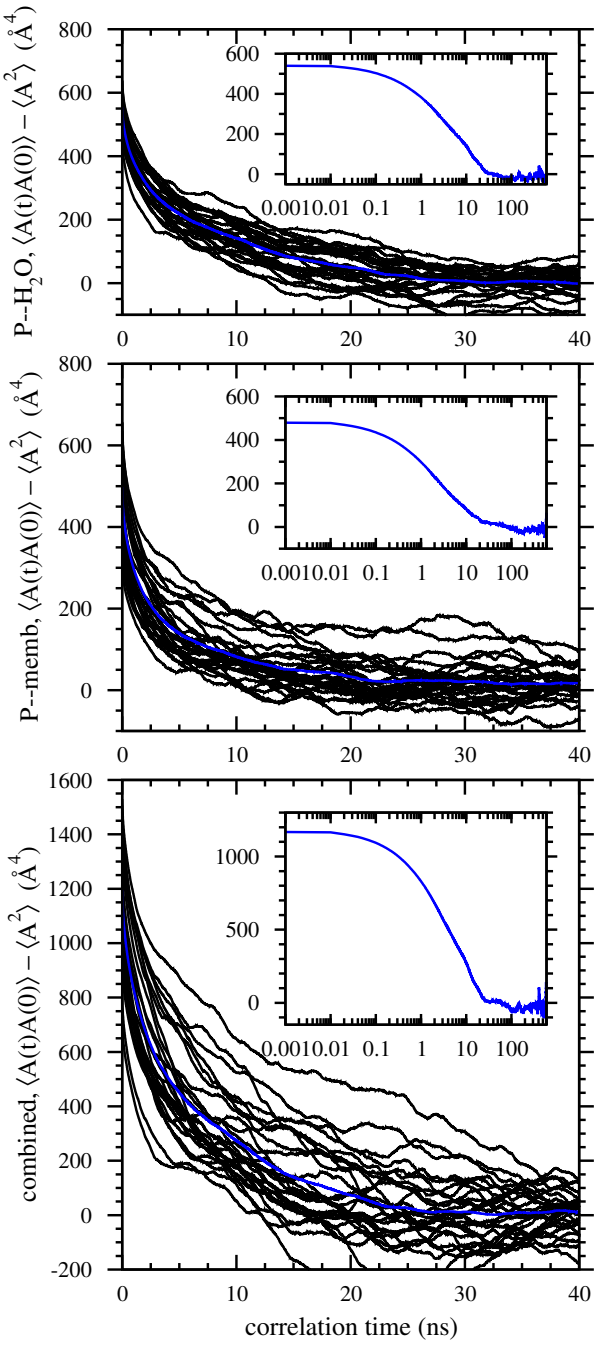

Figure S19: Relaxation of the contributions made by LPG(a17:0/a15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the inner leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

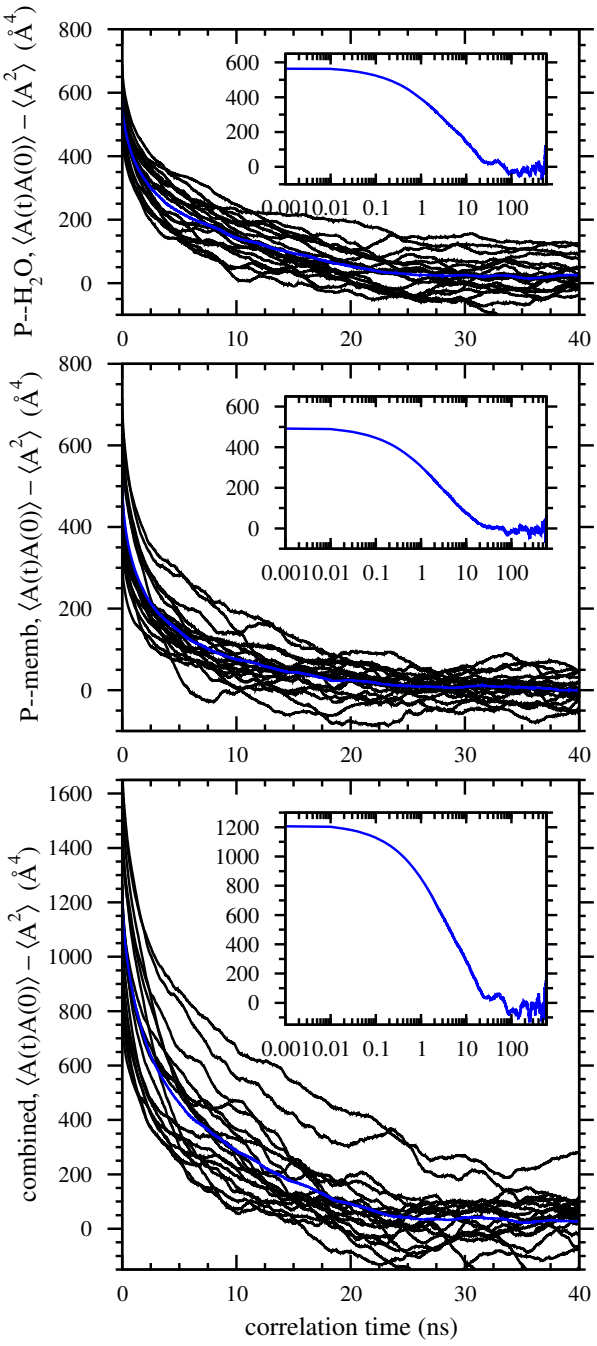

Figure S20: Relaxation of the contributions made by LPG(i17:0/a15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the inner leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

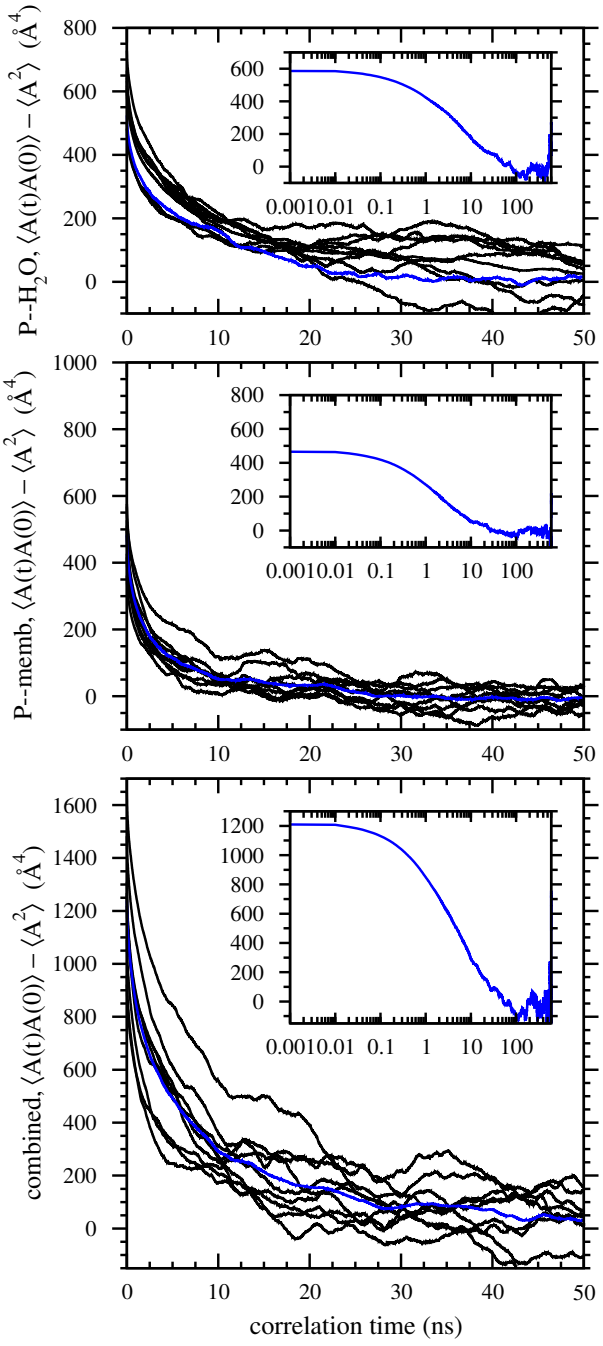

Figure S21: Relaxation of the contributions made by LPG(18:0/a15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the inner leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

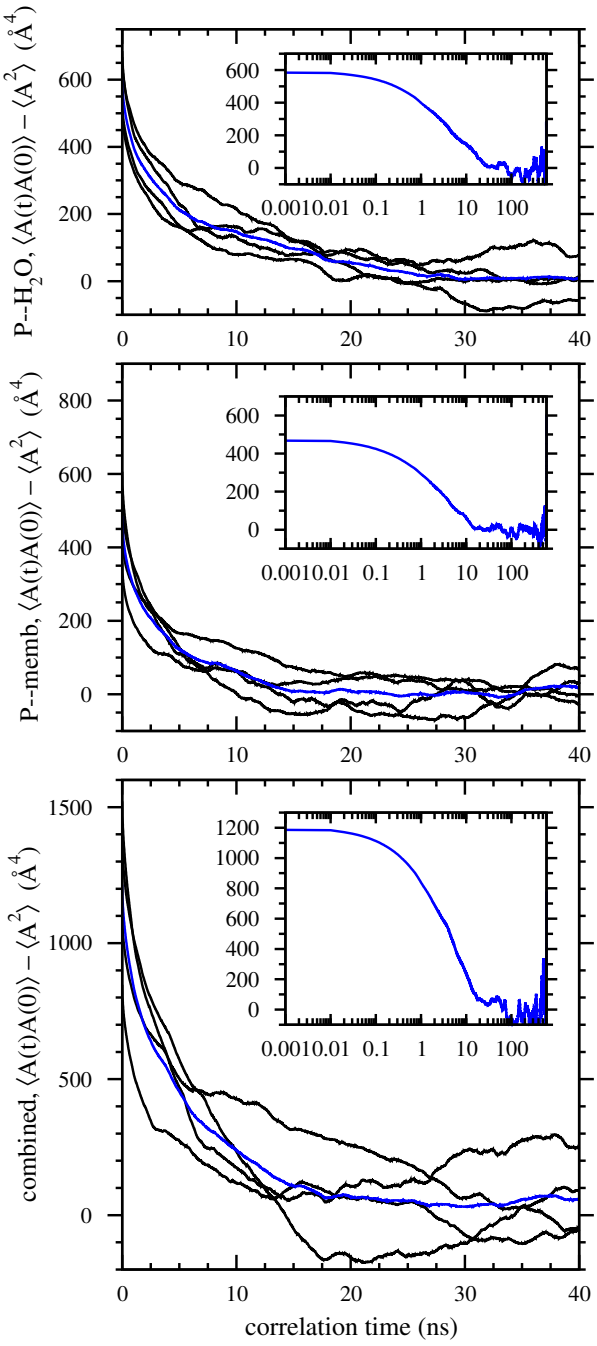

Figure S22: Relaxation of the contributions made by LPG(a19:0/a15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the inner leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

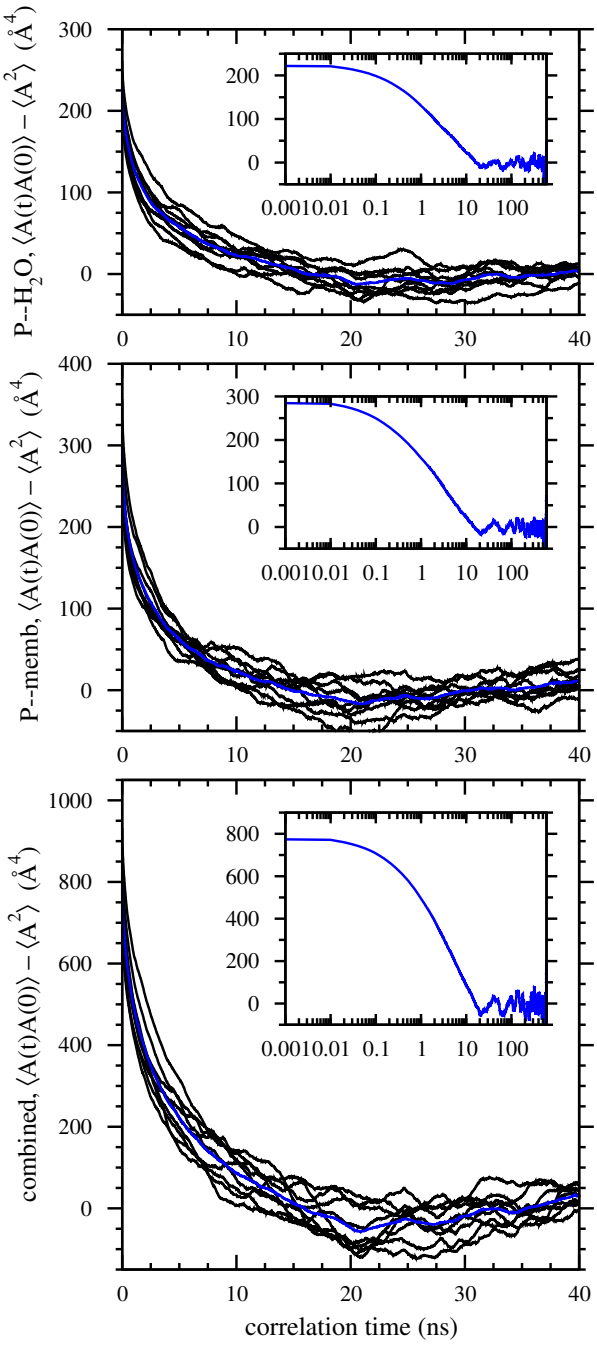

Figure S23: Relaxation of the contributions made by PG(a15:0/a15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the outer leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

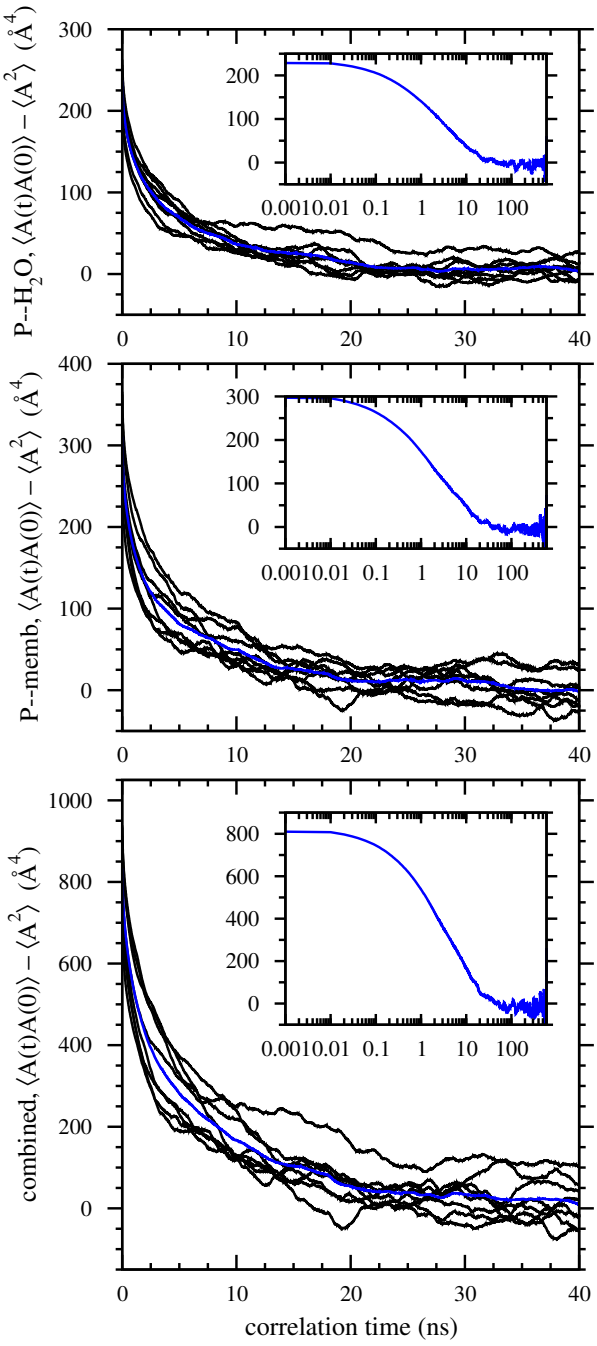

Figure S24: Relaxation of the contributions made by PG(i15:0/a15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the outer leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

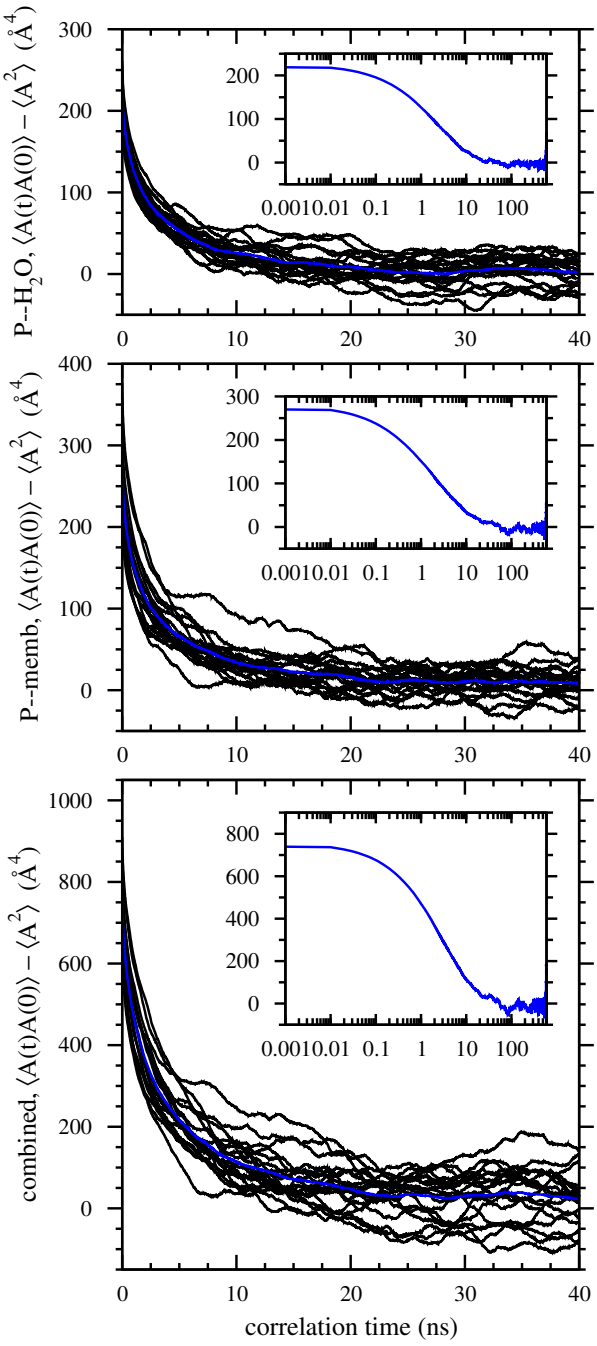

Figure S25: Relaxation of the contributions made by PG(16:0/a15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the outer leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

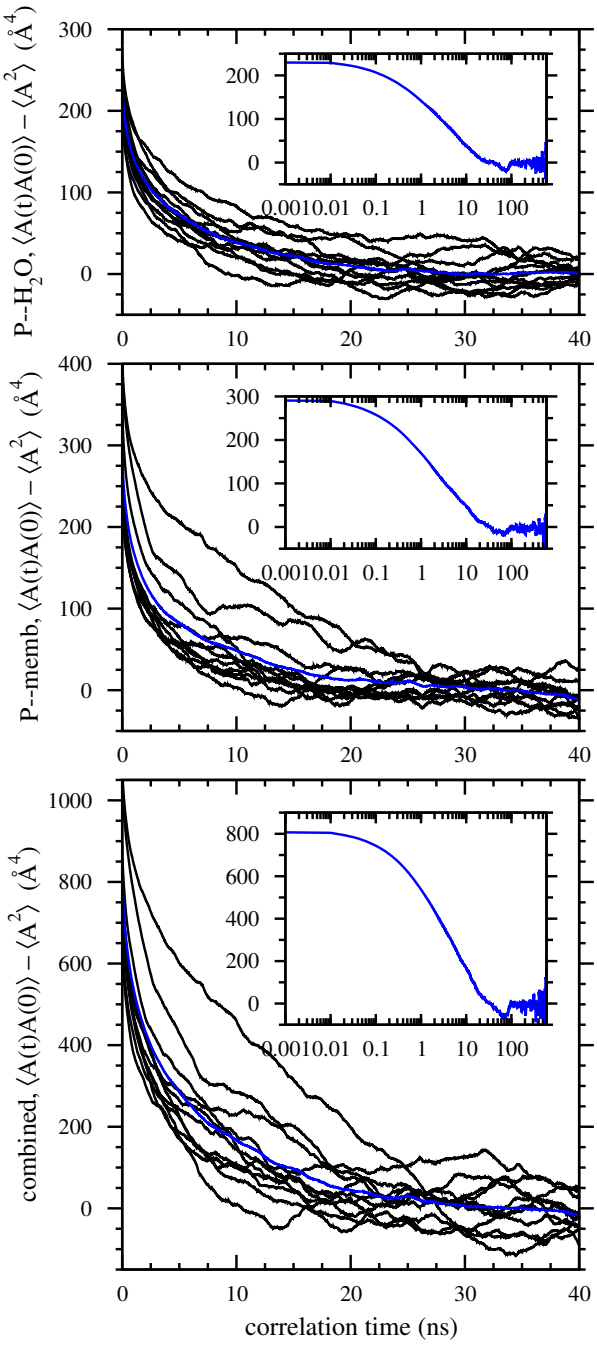

Figure S26: Relaxation of the contributions made by PG(a17:0/a15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the outer leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

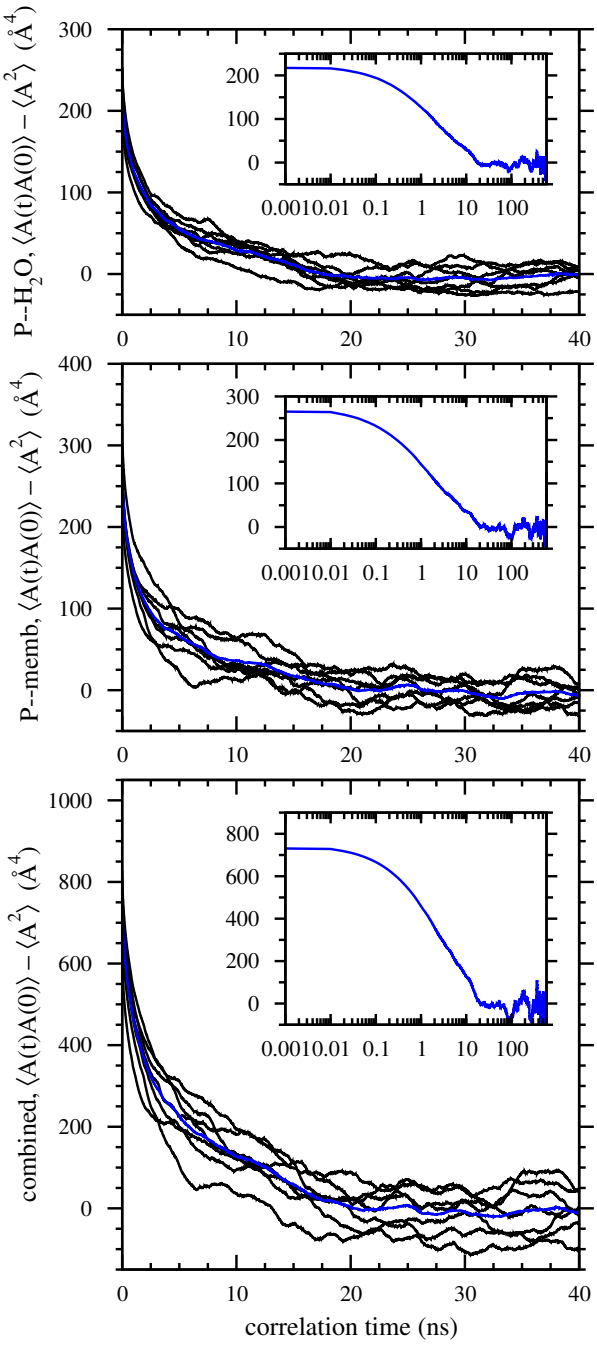

Figure S27: Relaxation of the contributions made by PG(i17:0/a15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the outer leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

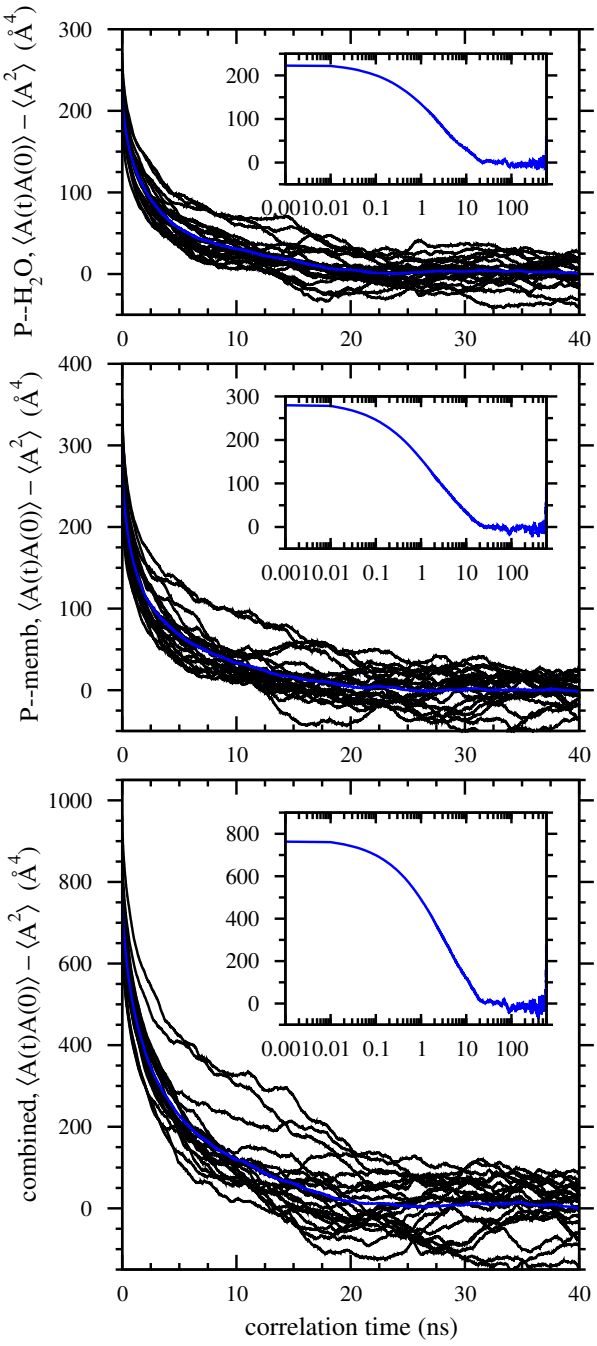

Figure S28: Relaxation of the contributions made by PG(a17:0/i15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the outer leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

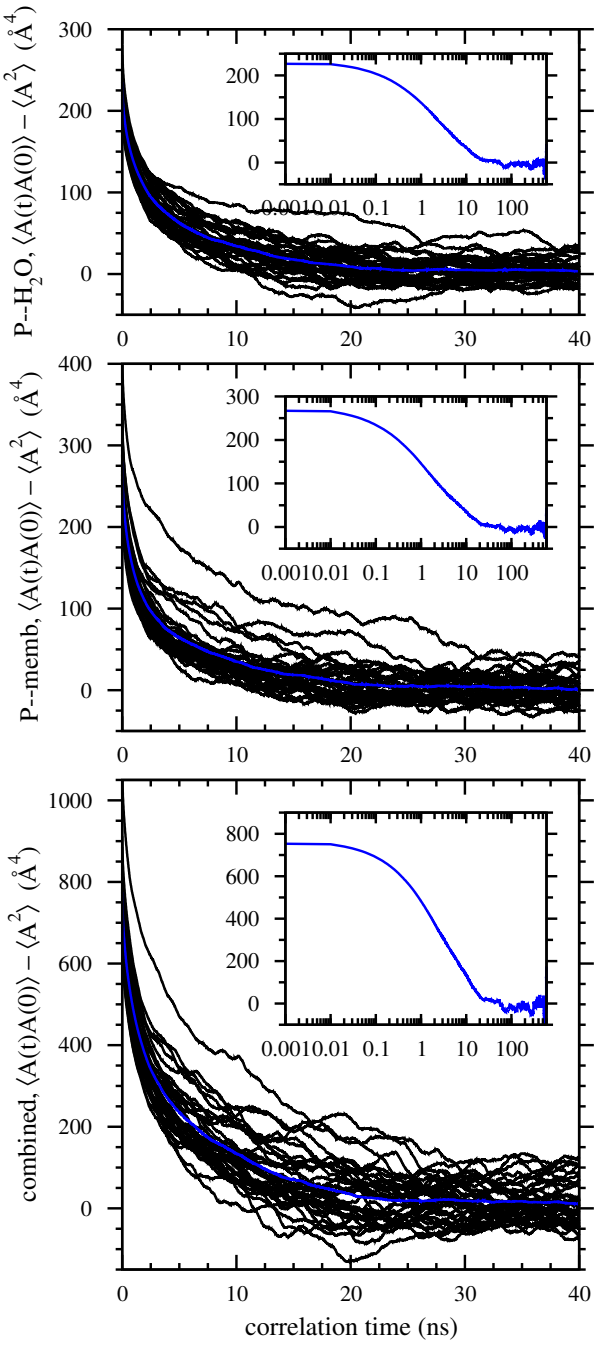

Figure S29: Relaxation of the contributions made by PG(i17:0/i15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the outer leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

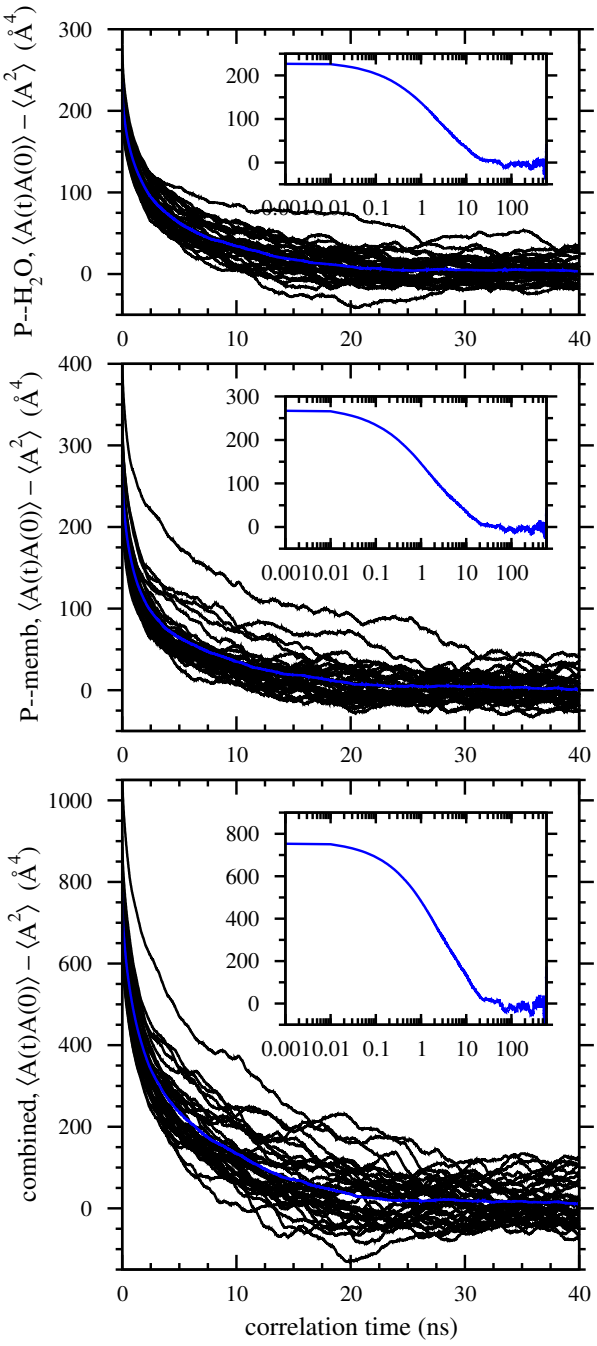

Figure S30: Relaxation of the contributions made by PG(18:0/a15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the outer leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

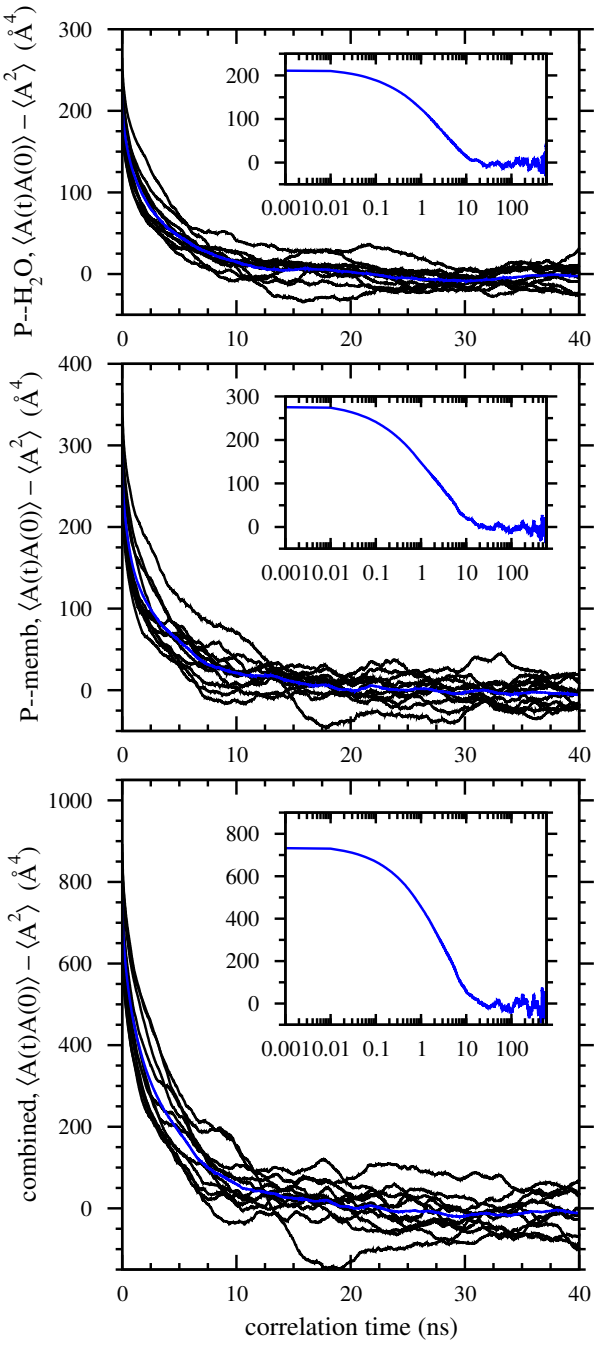

Figure S31: Relaxation of the contributions made by PG(18:1/a15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the outer leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

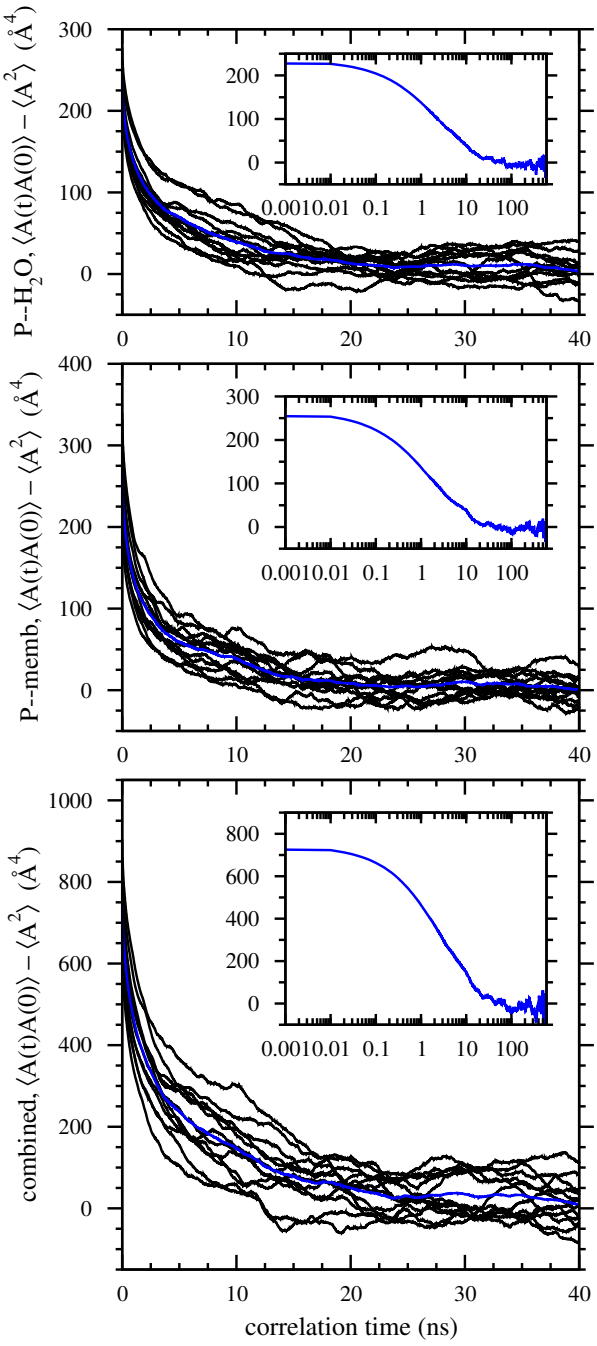

Figure S32: Relaxation of the contributions made by PG(18:1/i15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the outer leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

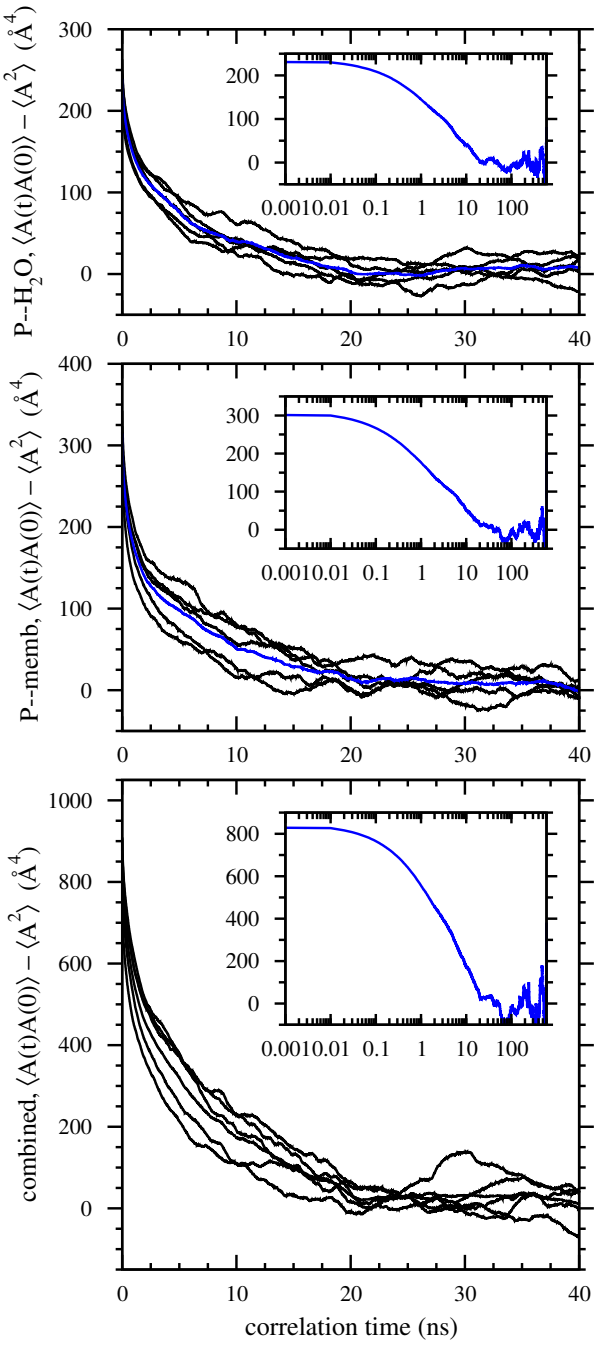

Figure S33: Relaxation of the contributions made by PG(a19:0/a15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the outer leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

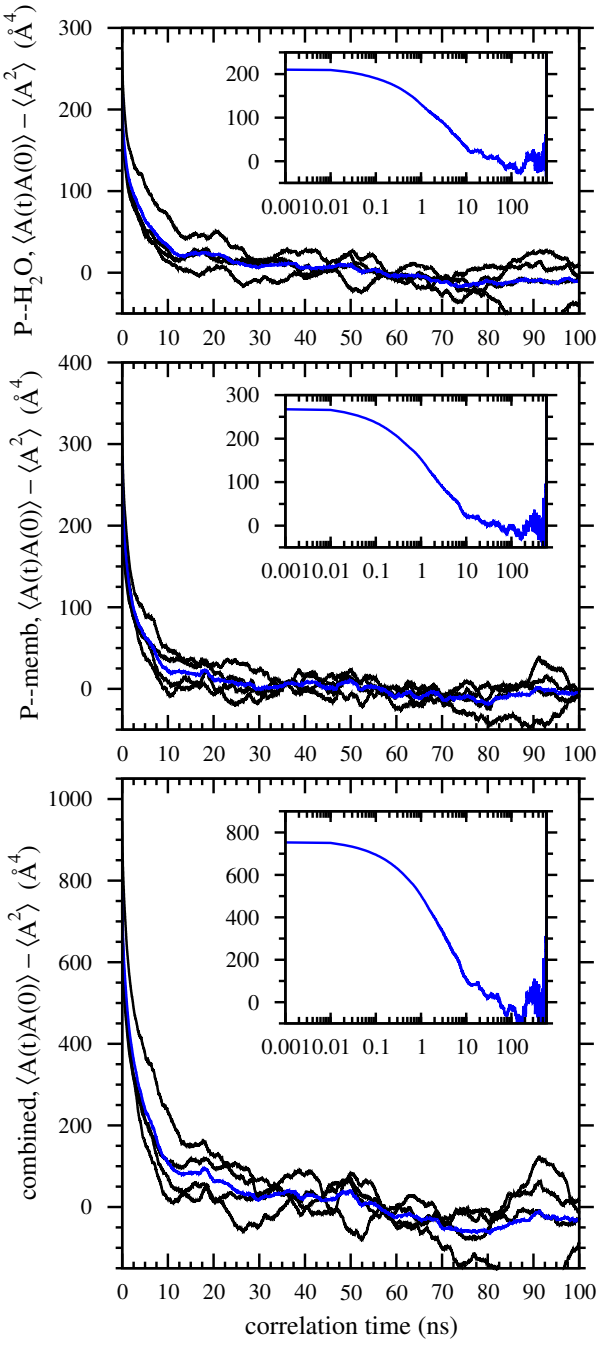

Figure S34: Relaxation of the contributions made by PG(i19:0/a15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the outer leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

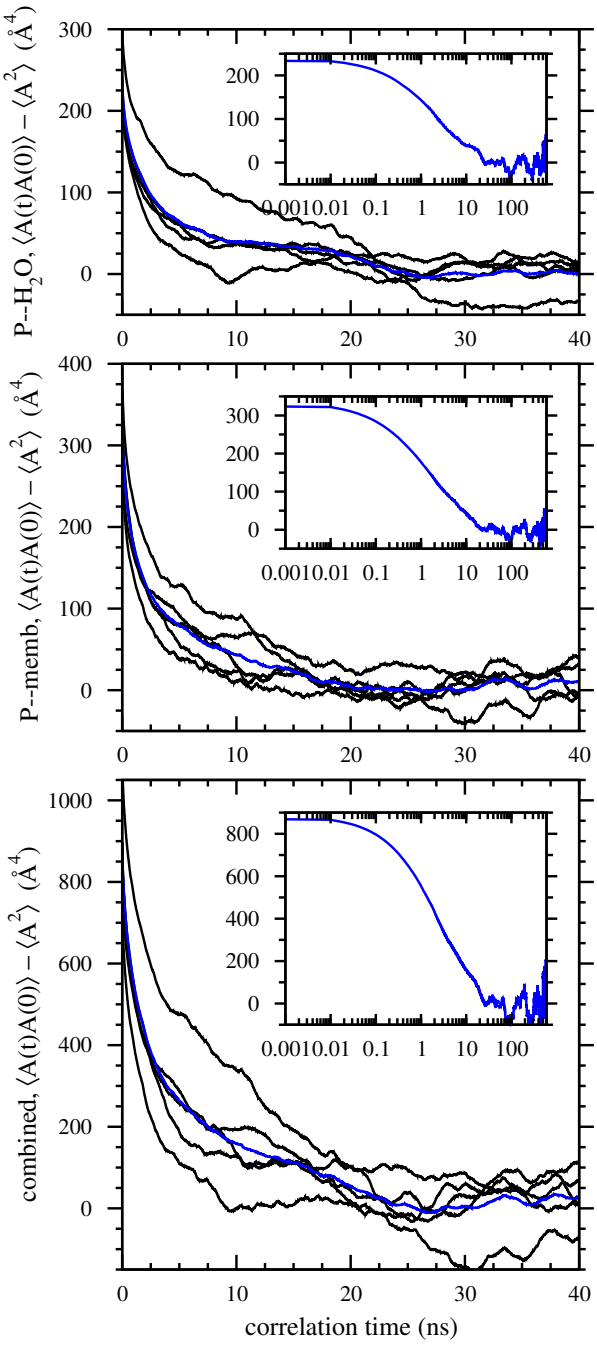

Figure S35: Relaxation of the contributions made by PG(a19:0/i15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the outer leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

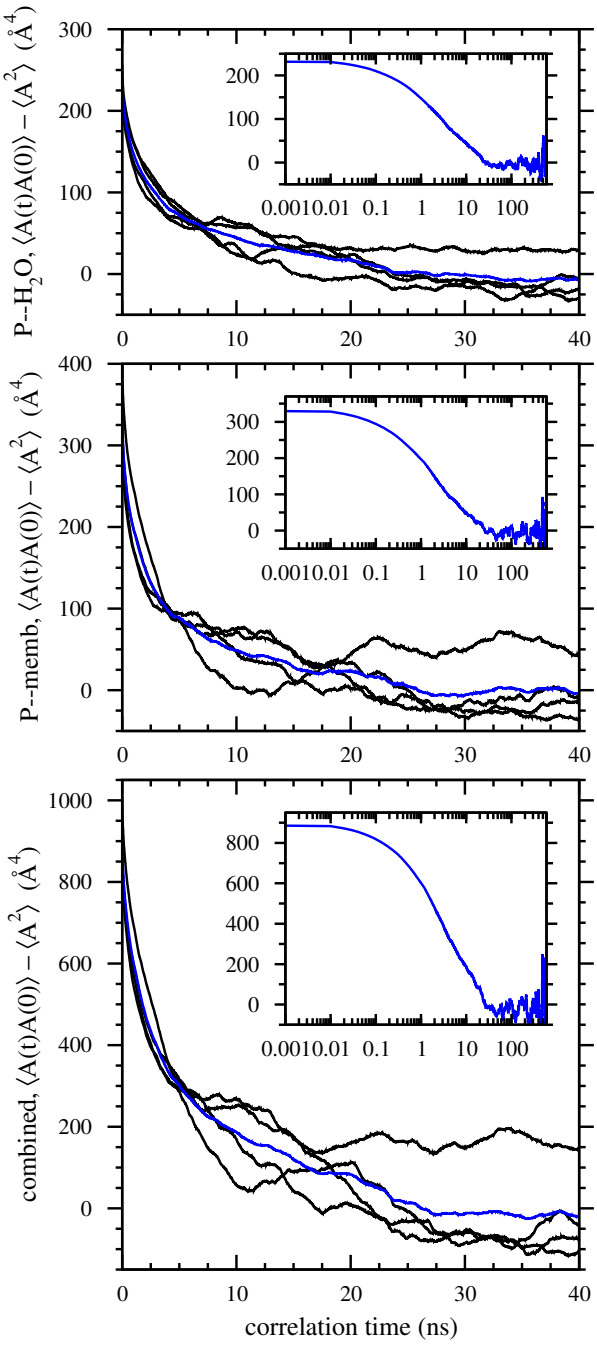

Figure S36: Relaxation of the contributions made by PG(20:0/a15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the outer leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

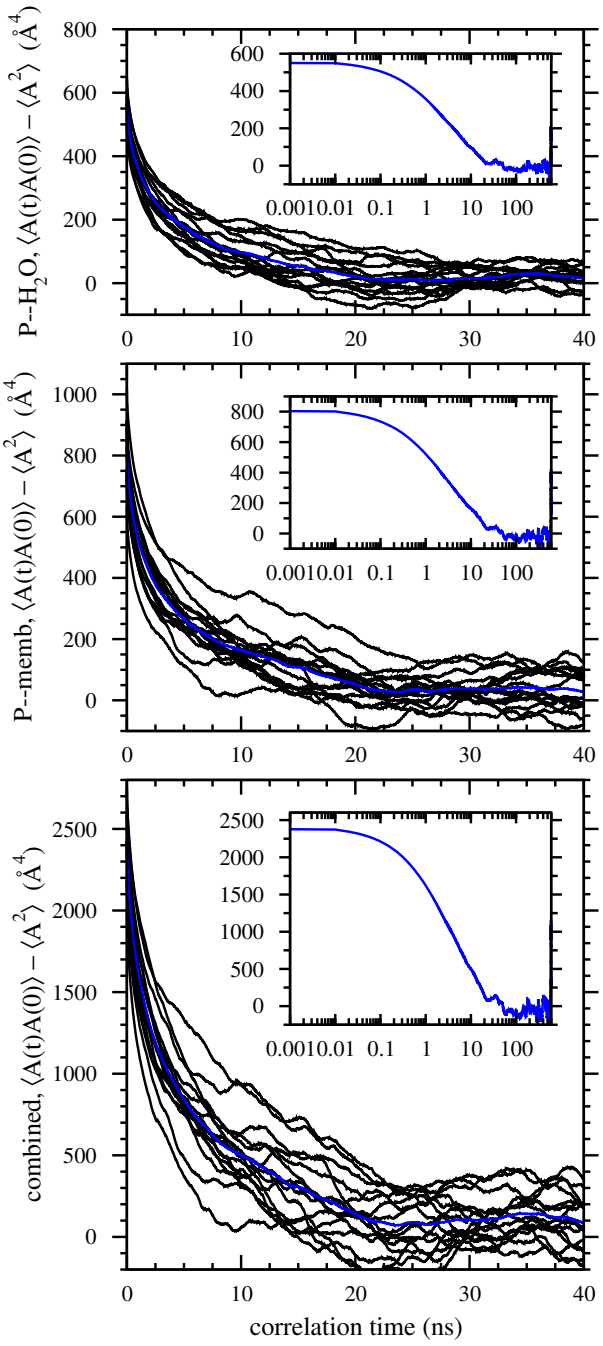

Figure S37: Relaxation of the contributions made by CL(a17:0/a15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the outer leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.

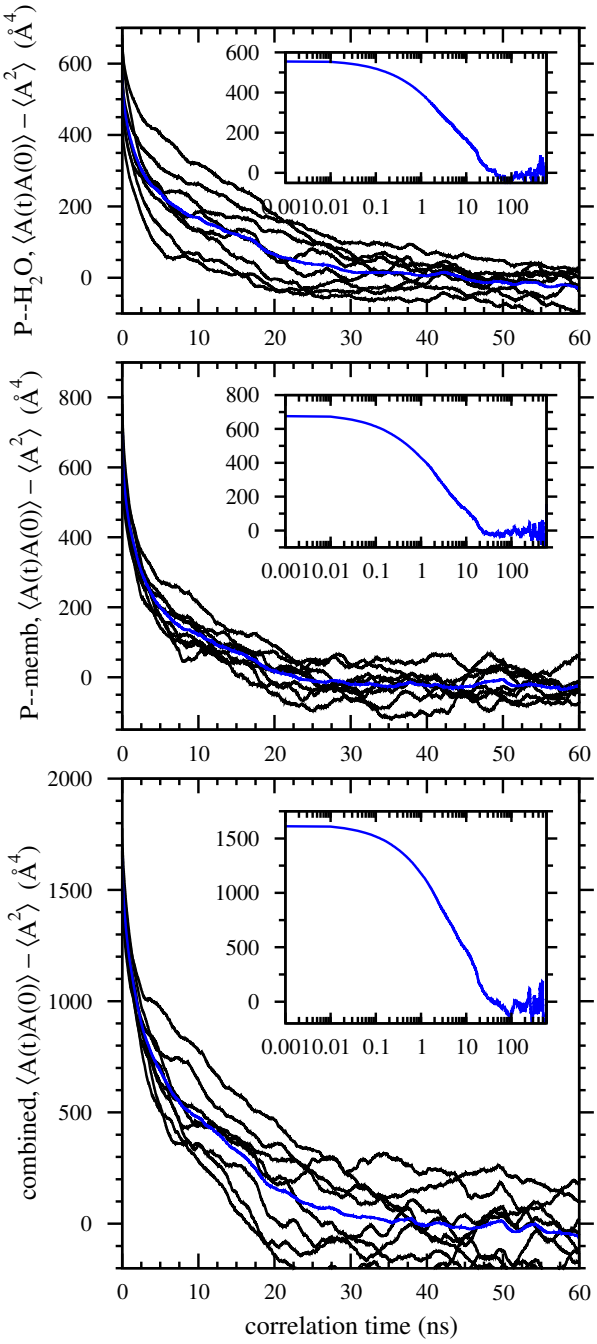

Figure S38: Relaxation of the contributions made by LPG(a17:0/a15:0) lipids to interfacial area in (a) a 5 Å-thick region between P atoms and water in the outer leaflet, (b) a 5 Å-thick region between P atoms and the membrane, and (c) both regions combined. Black lines depict relaxations of individual molecules; the thicker blue curve shows the average. Insets in (a, b, and c) depict average curves on a logarithmic time scale.