Supplementary Materials

Revisiting the Bilayer Structures of Fluid Phase Phosphatidylglycerol Lipids: Accounting for Exchangeable Hydrogens

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The structural parameters listed in the following tables include: (1) V_L and V_{HL} are the total lipid and headgroup volumes, respectively; (2) A is lipid area; (3) D_B, $2D_C$, and D_{HH} are the overall bilayer thickness, bilayer hydrocarbon chain thickness, and the distance between electron density maxima, respectively; (4) D_{H1} is characteristic distance calculated from $D_{H1}= D_{HH}/2-D_C$; (5) z_{G1}, σ_{G1} and R_{G1} are, respectively, the Gaussian center, width and volume fraction with respect to the total headgroup of the G1 component. The same annotation was applied to the G2 and G3 components (*i.e.,* z_{G2}, σ_{G2}, R_{G2}, and z_{G3}, σ_{G3}, R_{G3}); (6) z_{HC} and σ_{HC} are, respectively, the half-length (the same as D_C) and width of the error function representing the total hydrocarbon chain region; (7) σ_{CH3} and r_{CH3} are, respectively, the Gaussian width and volume ratio of V_{CH3}/V_{CH2}, where V_{CH3} and V_{CH2} refer to the CH3 and CH2 volumes divided by the number of non-hydrogen atoms (carbons) in each group; (8) similar to r_{CH3}, r_{12} is the volume ratio of V_{CH}/V_{CH2}, where V_{CH} is the average CH group volume.

To facilitate data analysis, V_L and V_{HL} were fixed to values obtained from experiment. In addition, several parameters were "softly" constrained to values obtained from MD simulations [S1, S2]. They include R_{G1} (0.51) and R_{G2} (0.16), r_{CH3} (1.8), r_{12} (0.64), z_{CH} (7.5), σ_{CH} (3.2), σ_{HC} (2.65), and σ_{G3} (3.2) with target values given in parentheses.

Table S1. Structural parameters of DOPG bilayers from SDP model analysis.

T (^{o}C)	20	30	50	60
V_L (Å^3)	1257.5	1265.0	1281.0	1288.2
V_{HL} (Å^3)	291.0	291.0	291.0	291.0
R_{G1}	0.45	0.47	0.47	0.45
R_{G2}	0.16	0.16	0.16	0.16
r_{CH3}	1.61	1.73	1.80	1.83
r_{12}	0.64	0.64	0.64	0.63
D_B (Å)	37.1	36.6	36.0	35.9
D_{HH} (Å)	35.8	35.8	35.4	35.6
$2D_C$ (Å)	28.5	28.2	27.8	27.8
DH_1 (Å)	3.7	3.8	3.8	3.9
A (Å^2)	67.9	69.1	71.1	71.7
z_{G1} (Å)	14.7	14.6	14.4	14.2
σ_{G1} (Å)	2.5	2.5	2.5	2.5
z_{G2} (Å)	18.9	18.8	18.6	18.7
σ_{G2} (Å)	2.7	2.7	2.7	2.7
z_{G3} (Å)	18.9	18.8	18.6	18.7
σ_{G3} (Å)	3.1	3.2	3.2	3.1
z_{CH} (Å)	6.6	7.1	7.3	7.2
σ_{CH} (Å)	3.1	3.2	3.1	2.8
σ_{HC} (Å)	2.7	2.7	2.7	2.7
σ_{CH3} (Å)	3.7	3.7	3.6	3.6

Table S2. Structural parameters of POPG bilayers from SDP model analysis.

T (^{o}C)	20	30	50	60
V (Å^3)	1201.9	1208.7	1233.7	1243.6
V_{HL} (Å^3)	291.0	291.0	291.0	291.0
R_{G1}	0.49	0.50	0.50	0.50
R_{G2}	0.16	0.16	0.16	0.16
r_{CH3}	1.76	1.82	1.88	1.91
r_{12}	0.62	0.63	0.63	0.63
D_B (Å)	38.5	37.6	36.1	35.7
D_{HH} (Å)	37.0	36.6	35.6	35.4
$2D_C$ (Å)	29.1	28.5	27.6	27.4
DH_1 (Å)	3.9	4.0	4.0	4.0
A (Å^2)	62.5	64.3	68.4	69.6
z_{G1} (Å)	15.2	14.9	14.3	14.1
σ_{G1} (Å)	2.6	2.6	2.5	2.5
z_{G2} (Å)	18.9	18.7	18.2	18.1
σ_{G2} (Å)	2.7	2.7	2.7	2.7
z_{G3} (Å)	21.9	21.5	21.2	21.0
σ_{G3} (Å)	3.2	3.2	3.1	3.1
z_{CH} (Å)	7.0	7.2	7.4	7.4
σ_{CH} (Å)	2.7	2.9	3.0	2.9
σ_{HC} (Å)	2.7	2.7	2.7	2.7
σ_{CH3} (Å)	3.6	3.5	3.5	3.4

Table S3. Structural parameters of SOPG bilayers from SDP model analysis.

T (^{o}C)	20	30	50	60
V (Å^3)	1265.5	1272.8	1288.6	1297.1
V_{HL} (Å^3)	291.0	291.0	291.0	291.0
R_{G1}	0.47	0.48	0.50	0.50
R_{G2}	0.15	0.15	0.16	0.16
r_{CH3}	1.63	1.78	1.89	1.92
r_{12}	0.58	0.62	0.63	0.63
D_B (Å)	40.2	39.6	38.1	37.6
D_{HH} (Å)	38.8	38.2	37.2	36.6
$2D_C$ (Å)	31.0	30.5	29.5	29.2
DH_1 (Å)	3.9	3.8	3.8	3.7
A (Å^2)	62.9	64.3	67.6	69.0
z_{G1} (Å)	16.2	16.0	15.3	15.2
σ_{G1} (Å)	2.8	2.7	2.6	2.6
z_{G2} (Å)	19.9	19.6	19.0	18.7
σ_{G2} (Å)	2.6	2.6	2.7	2.7
z_{G3} (Å)	23.5	23.5	22.0	22.2
σ_{G3} (Å)	3.2	3.2	3.2	3.2
z_{CH} (Å)	6.7	7.1	7.5	7.5
σ_{CH} (Å)	2.7	2.7	3.0	3.0
σ_{HC} (Å)	2.8	2.7	2.7	2.7
σ_{CH3} (Å)	3.4	3.5	3.5	3.4

Table S4. Structural parameters of DLPG bilayers from SDP model analysis.

T (^{o}C)	20	30	50	60
V (Å^3)	945.9	953.6	962.4	971.5
V_{HL} (Å^3)	291.0	291.0	291.0	291.0
R_{G1}	0.50	0.49	0.50	0.50
R_{G2}	0.16	0.16	0.16	0.16
r_{CH3}	1.81	1.85	1.88	1.94
r_{12}	NA	NA	NA	NA
D_B (Å)	31.4	30.7	29.5	28.9
D_{HH} (Å)	30.0	29.4	28.8	28.4
$2D_C$ (Å)	21.7	21.3	20.6	20.3
DH_1 (Å)	4.1	4.0	4.1	4.1
A (Å^2)	60.2	62.1	65.3	67.1
z_{G1} (Å)	11.6	11.3	10.9	10.8
σ_{G1} (Å)	2.6	2.6	2.6	2.6
z_{G2} (Å)	15.7	15.5	15.1	15.0
σ_{G2} (Å)	2.9	2.9	2.9	3.0
z_{G3} (Å)	16.5	16.1	15.7	15.6
σ_{G3} (Å)	3.1	3.2	3.2	3.3
z_{CH} (Å)	NA	NA	NA	NA
σ_{CH} (Å)	NA	NA	NA	NA
σ_{HC} (Å)	2.8	2.8	2.7	2.7
σ_{CH3} (Å)	3.5	3.5	3.4	3.3

Table S5. Structural parameters of DMPG bilayers from SDP model analysis.

T (^{o}C)	30	50	60
V (Å^3)	1057.4	1074.0	1080.9
V_{HL} (Å^3)	291.0	291.0	291.0
R_{G1}	0.49	0.49	0.49
R_{G2}	0.16	0.16	0.16
r_{CH3}	1.60	1.98	1.99
r_{12}	NA	NA	NA
D_B (Å)	33.8	32.6	32.0
D_{HH} (Å)	34.6	34.6	33.8
$2D_C$ (Å)	24.5	23.7	23.4
DH_1 (Å)	5.0	5.4	5.2
A (Å^2)	62.5	66.0	67.5
z_{G1} (Å)	12.9	12.3	12.1
σ_{G1} (Å)	2.5	2.5	2.5
z_{G2} (Å)	17.8	17.6	17.2
σ_{G2} (Å)	2.8	2.6	2.7
z_{G3} (Å)	18.4	18.0	17.7
σ_{G3} (Å)	3.3	3.1	3.1
z_{CH} (Å)	NA	NA	NA
σ_{CH} (Å)	NA	NA	NA
σ_{HC} (Å)	2.7	2.7	2.7
σ_{CH3} (Å)	3.7	3.5	3.5

Table S6. Structural parameters of DPPG bilayers from SDP model analysis.

T (^{o}C)	50	60
V (Å^3)	1188.8	1198.1
V_{HL} (Å^3)	291.0	291.0
R_{G1}	0.49	0.49
R_{G2}	0.16	0.16
r_{CH3}	1.87	1.95
r_{12}	NA	NA
D_B (Å)	36.7	35.9
D_{HH} (Å)	38.6	37.6
$2D_C$ (Å)	27.7	27.2
DH_1 (Å)	5.4	5.2
A (Å^2)	64.7	66.8
z_{G1} (Å)	14.4	14.0
σ_{G1} (Å)	2.7	2.5
z_{G2} (Å)	19.6	19.2
σ_{G2} (Å)	2.4	2.8
z_{G3} (Å)	20.1	19.7
σ_{G3} (Å)	3.0	3.2
z_{CH} (Å)	NA	NA
σ_{CH} (Å)	NA	NA
σ_{HC} (Å)	2.8	2.7
σ_{CH3} (Å)	3.5	3.6

Table S7. Structural parameters of DSPG bilayers from SDP model analysis.

$T\ (^oC)$	60
$V\ (Å^3)$	1305.0
$V_{HL}\ (Å^3)$	291.0
R_{G1}	0.48
R_{G2}	0.16
r_{CH3}	1.90
r_{12}	NA
$D_B\ (Å)$	39.1
$D_{HH}\ (Å)$	41.2
$2D_C\ (Å)$	30.4
$DH_1\ (Å)$	5.4
$A\ (Å^2)$	66.8
$z_{G1}\ (Å)$	15.8
$\sigma_{G1}\ (Å)$	2.6
$z_{G2}\ (Å)$	20.9
$\sigma_{G2}\ (Å)$	2.6
$z_{G3}\ (Å)$	21.6
$\sigma_{G3}\ (Å)$	3.1
$z_{CH}\ (Å)$	NA
$\sigma_{CH}\ (Å)$	NA
$\sigma_{HC}\ (Å)$	2.7
$\sigma_{CH3}\ (Å)$	3.4

References

[S1] N. Kučerka, B.W. Holland, C.G. Gray, B. Tomberli, J. Katsaras, Scattering Density Profile Model of POPG Bilayers As Determined by Molecular Dynamics Simulations and Small-Angle Neutron and X-ray Scattering Experiments, J Phys Chem B, 116 (2012) 232-239.

[S2] J.J. Pan, F.A. Heberle, S. Tristram-Nagle, M. Szymanski, M. Koepfinger, J. Katsaras, N. Kucerka, Molecular structures of fluid phase phosphatidylglycerol bilayers as determined by small angle neutron and X-ray scattering, BBA-Biomembranes, 1818 (2012) 2135-2148.