A computer model of a polyunsaturated monogalactolipid bilayer

(**Supplementary Material**)

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Equilibration and stability of the simulated bilayers

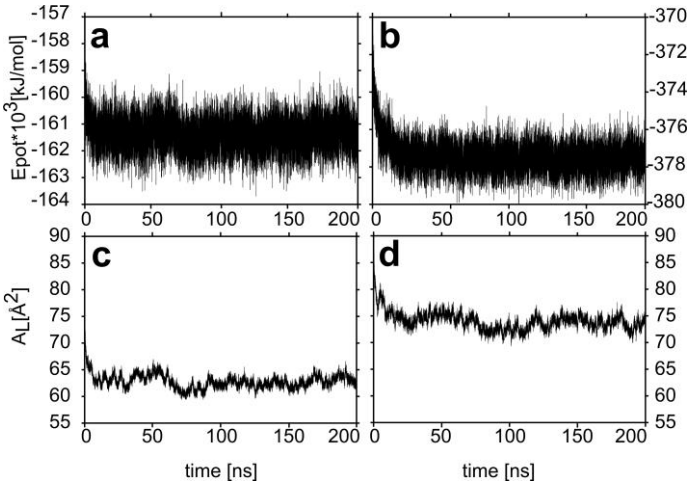

Figure S1. Time profiles of the potential energy, Epot (a, b), and the average cross-sectional area per lipid, A_L (c, d), for the MGDG (a, c) and DOPC (b, d) bilayers at 295 K in the range 0-200 ns.

Additionally, to check the stability of the lamellar phase of the MGDG and DOPC bilayers (main text), their simulations at 295 K were extended to 450 ns (cf., main text) and three time averaged values of A_L and the bilayer thickness (D, for definition, see main text) were obtained from three trajectory fragments, 100-200, 200-325, and 325-450 ns and are compared in Table S1. As the values of A_L and D for each fragment are practically the same (within the standard deviation) (Table S1), one may assume that the lamellar phase of the MGDG bilayer at 295 K is stable on the 450 ns timescale; as expected, the lamellar phase of the DOPC bilayer is also stable. Additionally, the entries in Table S1 indicate, that the bilayers equilibrated within first 100 ns of MD simulation.

Table S1. Stability of membrane parameters

Fragment	MGDG		DOPC	
	A_L [Å^2]	D_{RR} [Å]	A_L [Å^2]	D_{PP} [Å]
100-200 ns	62.66 ± 0.88	41.30 ± 0.59	73.53 ± 1.15	38.19 ± 0.23
200-325 ns	62.06 ± 1.10	41.74 ± 0.53	73.22 ± 1.22	38.32 ± 0.25
325-450 ns	62.23 ± 0.95	41.70 ± 0.66	74.49 ± 1.37	37.84 ± 0.27

Time averaged values of the surface area per lipid (A_L) and bilayer thickness (D) measured as the distance between the average positions of the centers-of-masses of the galactose rings (D_{RR}, MGDG) and of the phosphorus P atoms (D_{PP}, DOPC), in the opposite bilayer leaflets of the MGDG and DOPC bilayers, respectively, MD simulated at 295 K at three time periods after equilibration. The errors are standard deviation estimates.

MD simulation of the POPC bilayer – additional validation of the used OPLS-AA parameters

To further evaluate applicability of the OPLS-AA force field to MD simulations of mono-unsaturated lipid bilayers, a pure 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphatidylcholine (POPC) bilayer was MD simulated for 130 ns at 310 K using the same parameters and software as those for the DOPC and MGDG bilayers (main text). For this bilayer, only an average surface area available to a POPC molecule in the bilayer, A_L, was compared with experimental values published in the literature.

The value of A_L for POPC in the POPC bilayer simulated for 130 ns at 310 K is 66.53 ± 0.65 Å^2 (time average between 80 and 130 ns). This value compares well with experimental values of 68.3 ± 1.5 Å^2 at 30°C [1]; 64.3 Å^2 at 30°C [2]; 66 Å^2 at 37°C [3].

Table S2. Spontaneous curvature of the DOPC monolayer

Calculation method	τ_1^m [kT/nm]	c_0^m [nm^{-1}]
Ollila at al. methodology [4] without restraints on any covalent bond	8.48	0.74
Ollila at al. methodology [4] with restraints on covalent bonds involving hydrogen atoms	–8.45	–0.73
[5, 6] implementation of Goetz-Lipowsky decompositions without restraints on any covalent bond	6.64	0.58
[5, 6] implementation of Goetz-Lipowsky decompositions with restraints on covalent bonds involving hydrogen atoms	-12.06	-1.05
[5, 6] implementation of central force decompositions without restraints on any covalent bond	7.44	0.65
[5, 6] implementation of central force decompositions with restraints on covalent bonds involving hydrogen atoms	-13.02	-1.13

The values of spontaneous curvature of the DOPC monolayer, c_0^m, calculated from the first integral moment, τ_1^m, of the lateral pressure profile using different methodologies. The bilayer bending rigidity modulus, κ^b, of 23 kT calculated for DOPC (Table 1, main text), was used.

References

1. N. Kucerka, S. Tristram-Nagle, J.F. Nagle, J. Membr. Biol., 208 (2005) 193-202.
2. N. Kucerka, M.P. Nieh, J. Katsaras, Biochim. Biophys. Acta-Biomem., 1808 (2011) 2761-2771.
3. R.P. Rand, V.A. Parsegian, Biochim. Biophys. Acta-Rev. Biomem., 988 (1989) 351-376.
4. O.H.S. Ollila, T. Rog, M. Karttunen, I. Vattulainen, J. Struct. Biol., 159 (2007) 311-323.
5. J.M. Vanegas, A. Torres-Sanchez, M. Arroyo, J. Chem. Theory Comput., 10 (2014) 691-702.
6. A. Torres-Sánchez, J.M. Vanegas, M. Arroyo, Phys. Rev. Lett., 114 (2015) 258102.