In Silico Design of Robust Bolalipid Membranes

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Supporting information for: *In-silico* design of

robust bolalipid membranes

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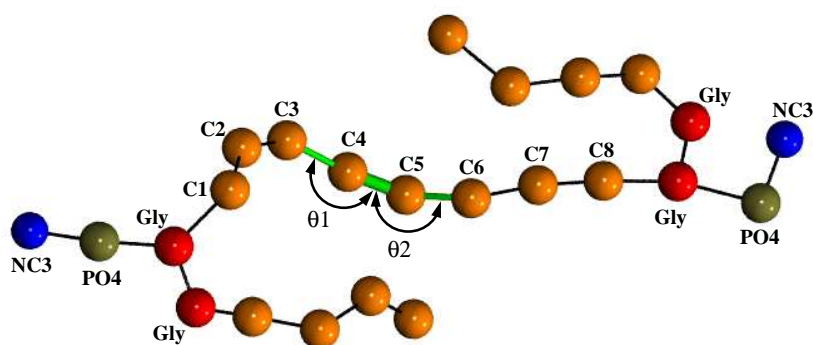
Figure 1: The coarse-grained model of a bola lipid (acyclic). Orange represents the methylene units, red the glycerol, blue the choline and tan the phosphate. The thick green bond is the covalent bond between the last beads from the tails of two DPPC lipids. Two bending potentials acting on the angles θ_1 and θ_2 control the linker stiffness (with equilibrium angle $\theta = 180°$ and $K = 25$ kJ mol^{-1}). Three cases are considered for the linker: stiff — bending potential on both angles, semi-flexible — only θ_1 is controlled, and flexible — both θ_1 and θ_2 are free.

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Table 1: Structural and dynamic properties of the bolalipid membranes: average fraction of trans conformers, area per lipid head group A, membrane thickness d_{PP}, and lipid lateral diffusion rate D. The (a) superscript refers to membranes in the gel phase, the (b) superscript to pre-assembled membranes with exclusively trans-conformations. The errors reported for A and d_{PP} are standard errors obtained by dividing each trajectory in independent blocks of 50 ns. The standard errors in D were obtained from the deviation between the five independent simulations for each type of system. Likewise, the standard error of the trans fraction is estimated around $2-3\%$.

system	linker type	trans [%]	T [K]	A [nm^2]	d_{PP} [nm]	D [$10^{-7}cm^2/s$]
DPPC	-	-	323	0.633 ± 0.001	4.13 ± 0.05	9.2 ± 0.2
	-	-	363	0.698 ± 0.001	3.94 ± 0.07	17.1 ± 0.2
acyclic di-DPPC						
	stiff	90	323	0.600 ± 0.001	4.25 ± 0.05	1.8 ± 0.1
	stiff[b]	100	323	0.593 ± 0.001	4.28 ± 0.04	2.0 ± 0.3
	semi-flexible	60	323	0.616 ± 0.002	4.19 ± 0.09	1.7 ± 0.1
	flexible	40	323	0.618 ± 0.002	4.16 ± 0.09	2.3 ± 0.4
cyclic di-DPPC						
	stiff[a]	96	363	0.568 ± 0.007	4.45 ± 0.11	0.2 ± 0.1
	stiff[a,b]	100	363	0.500 ± 0.004	4.60 ± 0.03	-
	semi-flexible	70	363	0.632 ± 0.001	4.15 ± 0.11	2.7 ± 0.2
	semi-flexible[a,b]	100	363	0.578 ± 0.003	4.38 ± 0.08	-
	flexible	40	323	0.603 ± 0.001	4.26 ± 0.10	0.9 ± 0.2