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Supplemental Information

Lipid Configurations from Molecular Dynamics Simulations

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Supporting Material

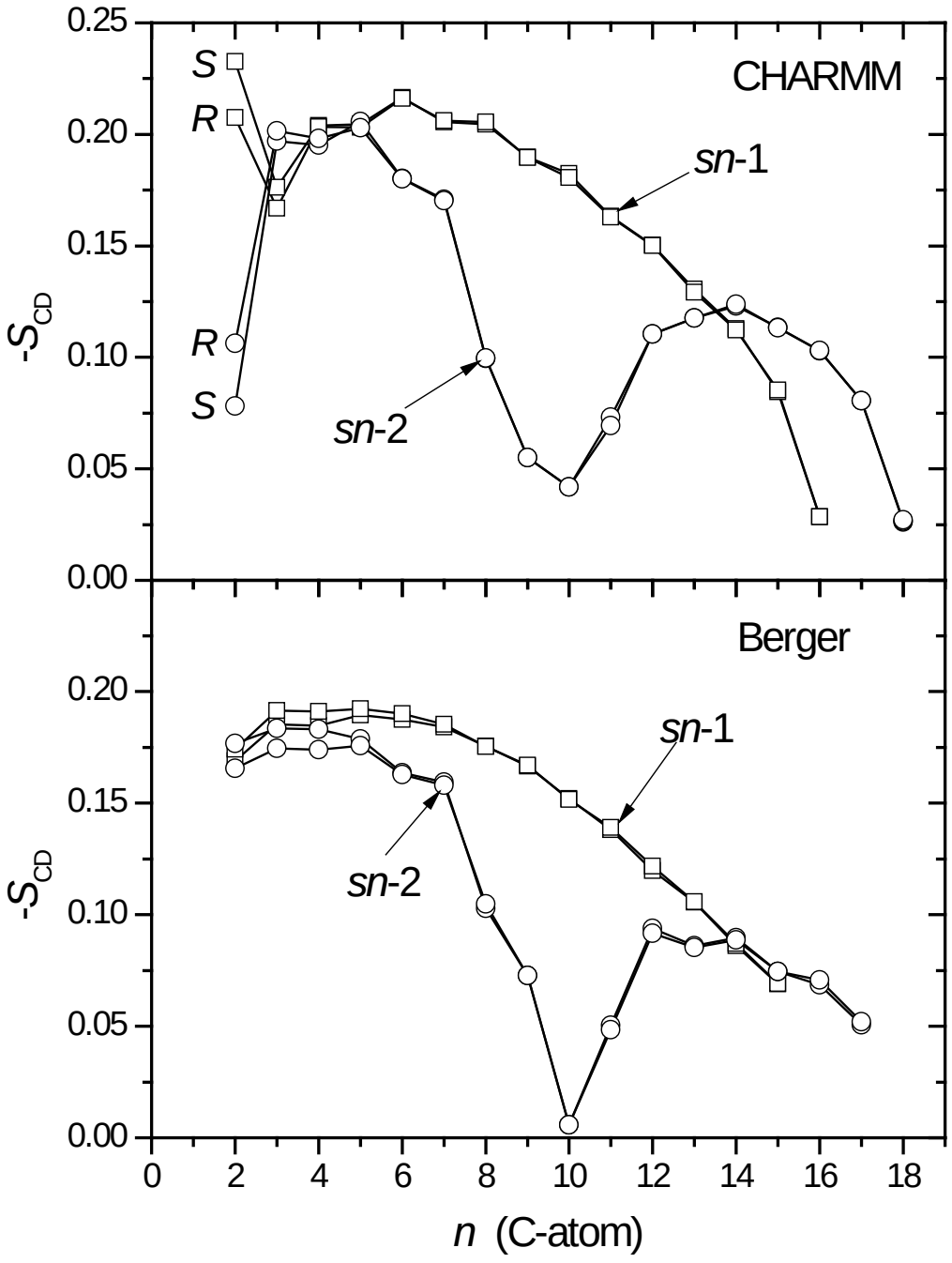

Fig. S.1 C–D order parameters of the *sn*-1 (squares) and *sn*-2 (circles) chains of POPC. MD simulations using the CHARMM36 (top panel) and Berger et al. (bottom panel) force fields. Prochirality (*R*,*S*) of the H-atoms on C2 is indicated.

Table S.1 Comparison of partial atomic charges for united atoms of the Berger et al. force field.

atom	CHARMM[a]	Berger et al.[b]	atom	CHARMM[a]	Berger et al.[b]
N	-0.60	-0.50	C2	0.26	0.30
C33,C34,C35	0.40	0.40	O21	-0.49	-0.70
C32	0.40	0.30	C21	0.90	0.70
C31	0.10	0.40	O22	-0.63	-0.70
P	1.50	1.70	C22	-0.04	0.00
O33,O34	-0.78	-0.80	C3	0.26	0.50
O32	-0.57	-0.80	O31	-0.49	-0.70
O31	-0.57	-0.70	C31	0.90	0.80
C3	0.10	0.40	O32	-0.63	-0.60
			C32	-0.04	0.00

[a] Net atomic charge in CHARMM36 (21) corresponding to the united atoms used for the force field of Berger et al. (20).
[b] Taken from quantum chemical calculations of Chiu et al. (24).