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Supplemental Information

Lipid Configurations from Molecular Dynamics Simulations

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Supporting Material

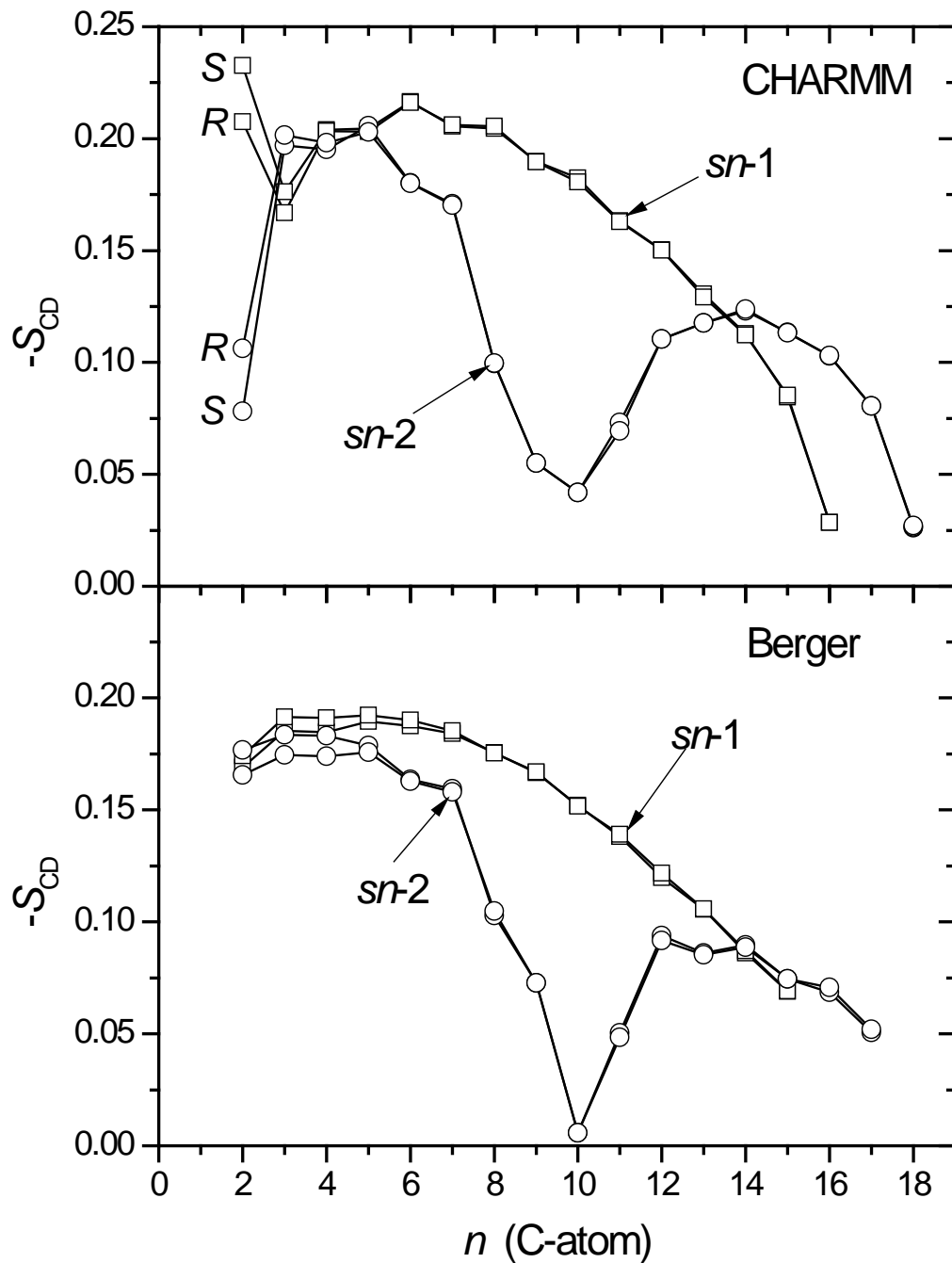


Fig. S.1 C–D order parameters of the $sn-1$ (squares) and $sn-2$ (circles) chains of POPC. MD simulations using the CHARMM36 (top panel) and Berger et al. (bottom panel) force fields. Prochirality (R,S) of the H-atoms on C2 is indicated.

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).