

Investigating the order parameters of saturated lipid molecules under various curvature conditions on spherical supported lipid bilayers

Lauren E. Marbella,^{†} Bocheng Yin,[†] Megan M. Spence*

Department of Chemistry, University of Pittsburgh, Pittsburgh, Pennsylvania 15260, United States

Supporting Information

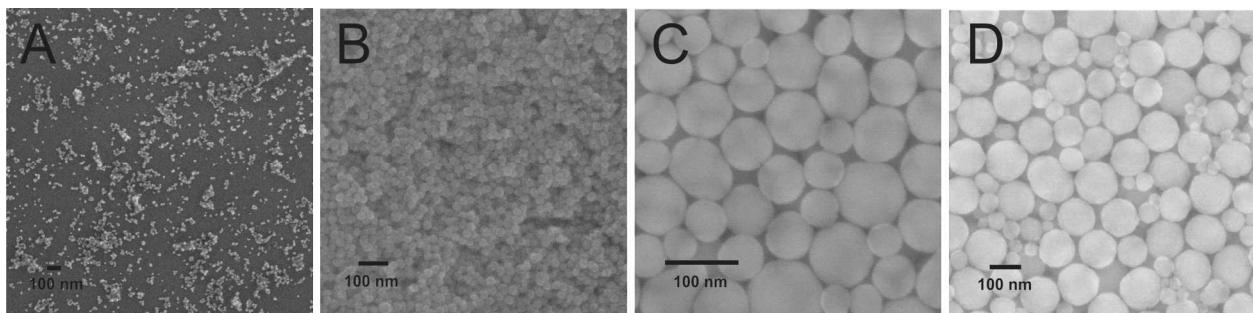


Figure S1. SEM of the raw SiO_2 beads as received A) $d = 10\text{-}20\text{ nm}$ (ST-40), B) $d = 20\text{-}30\text{ nm}$ (ST-50), C) $d = 40\text{-}50\text{ nm}$ (ST-OL), D) $d = 70\text{-}100\text{ nm}$ (ST-ZL). All of the beads exhibit pseudo-spherical particle shape and no differences in surface morphology are observed.

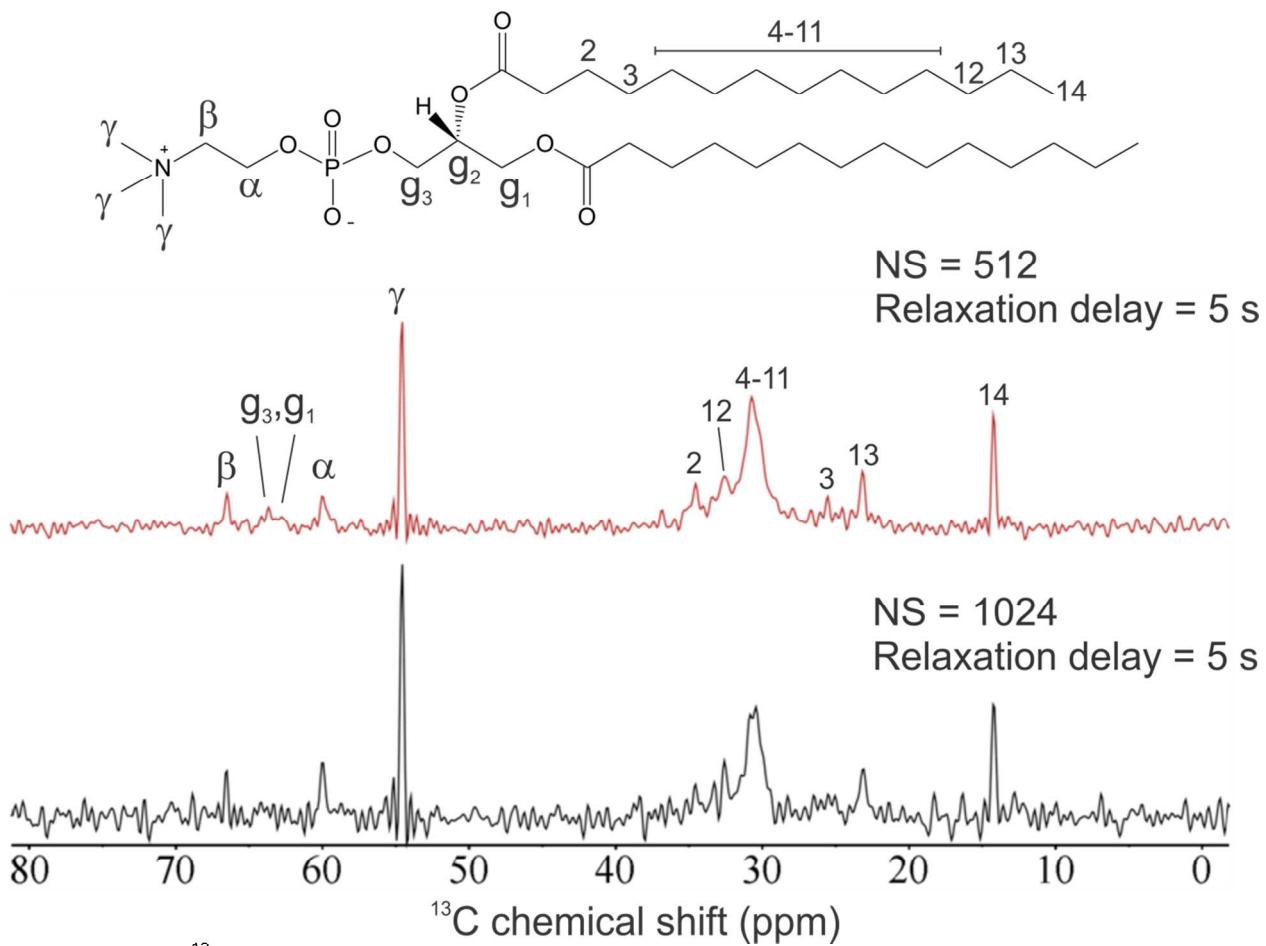


Figure S2. 1D ^{13}C direct polarization NMR for 30 nm LCBs acquired with 512 scans (top, red) and 100 nm unilamellar vesicles acquired with 1024 scans (bottom, black), labeled with the corresponding DMPC carbon sites. The 100 nm unilamellar vesicles showed the poorest signal-to-noise ratio of all the samples.

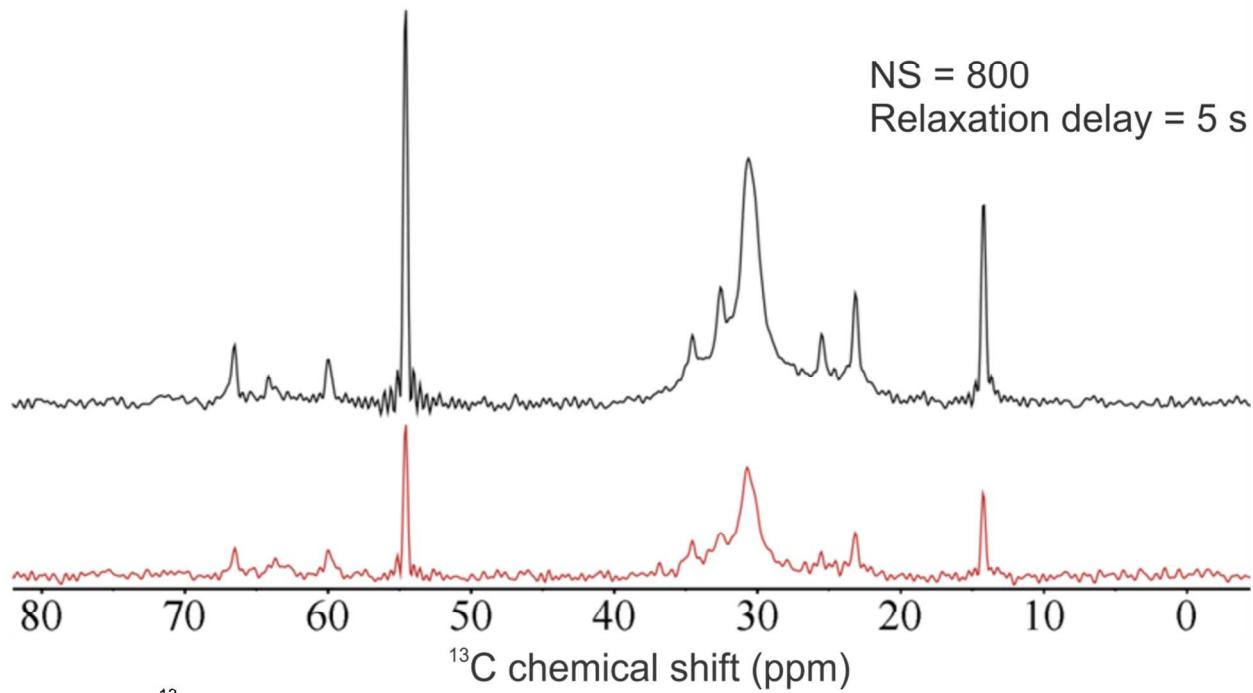


Figure S3. ¹³C NOE comparison spectra of 30 nm LCBs with presaturation (top, black) and without presaturation (bottom, red).

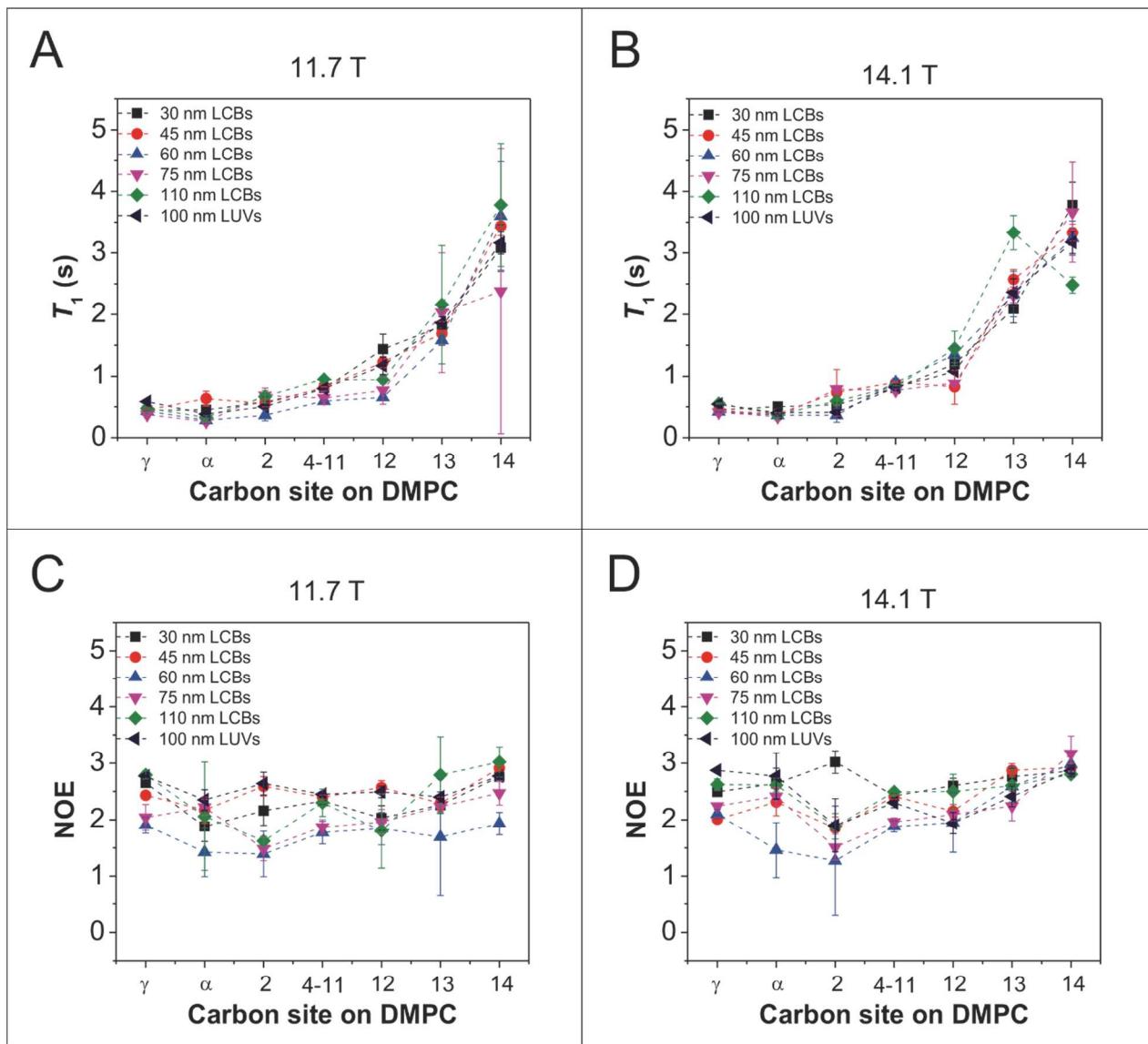


Figure S4. Raw T_1 data for various curvature conditions at 11.7 T (A) and 14.1 T (B). Raw NOE values for various curvature conditions at 11.7 T (C) and 14.1 T (D).

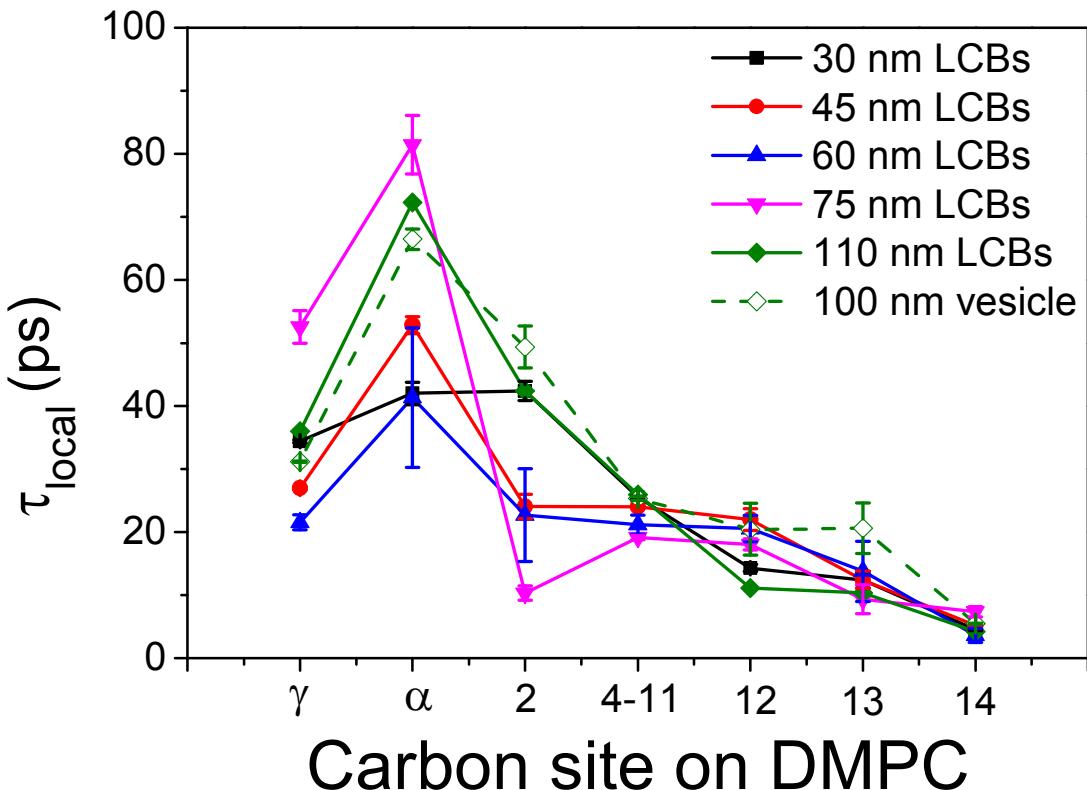


Figure S5. τ_{local} values as a function of carbon site on DMPC for various LCB sizes and 100 nm vesicles.

Table S1. Raw T_1 and NOE values for 30 nm LCBs at 11.7 T and 14.1 T

Carbon Site	11.7 T		14.1 T	
	T_1 (s)	NOE	T_1 (s)	NOE
γ	0.44 ± 0.01	2.65 ± 0.04	0.45 ± 0.01	2.49 ± 0.03
α	0.45 ± 0.05	1.88 ± 0.27	0.50 ± 0.02	2.64 ± 0.27
2	0.57 ± 0.09	2.16 ± 0.26	0.53 ± 0.03	3.02 ± 0.20
4-11	0.80 ± 0.02	2.33 ± 0.06	0.80 ± 0.01	2.42 ± 0.05
12	1.44 ± 0.24	2.03 ± 0.22	1.20 ± 0.13	2.60 ± 0.13
13	1.81 ± 0.31	2.26 ± 0.14	2.09 ± 0.23	2.76 ± 0.14
14	3.08 ± 0.38	2.76 ± 0.07	3.78 ± 0.37	2.86 ± 0.08

Table S2. Raw T_1 and NOE values for 45 nm LCBs at 11.7 T and 14.1 T

Carbon Site	11.7 T		14.1 T	
	T_1 (s)	NOE	T_1 (s)	NOE
γ	0.45 ± 0.02	2.43 ± 0.03	0.44 ± 0.01	2.01 ± 0.03
α	0.63 ± 0.12	2.17 ± 0.23	0.38 ± 0.01	2.31 ± 0.24
2	0.55 ± 0.05	2.59 ± 0.17	0.73 ± 0.38	1.85 ± 0.20
4-11	0.81 ± 0.01	2.40 ± 0.04	0.89 ± 0.01	2.41 ± 0.05
12	1.23 ± 0.09	2.57 ± 0.12	0.82 ± 0.28	2.15 ± 0.12
13	1.69 ± 0.19	2.29 ± 0.11	2.57 ± 0.16	2.87 ± 0.12
14	3.44 ± 0.16	2.91 ± 0.05	3.33 ± 0.14	2.92 ± 0.07

Table S3. Raw T_1 and NOE values for 60 nm LCBs at 11.7 T and 14.1 T

Carbon Site	11.7 T		14.1 T	
	T_1 (s)	NOE	T_1 (s)	NOE
γ	0.43 \pm 0.01	1.90 \pm 0.14	0.42 \pm 0.01	2.10 \pm 0.08
α	0.28 \pm 0.05	1.42 \pm 0.43	0.36 \pm 0.03	1.46 \pm 0.49
2	0.36 \pm 0.09	1.39 \pm 0.40	0.36 \pm 0.11	1.27 \pm 0.97
4-11	0.59 \pm 0.02	1.77 \pm 0.20	0.90 \pm 0.07	1.88 \pm 0.10
12	0.65 \pm 0.05	1.84 \pm 0.29	1.35 \pm 0.13	1.95 \pm 0.53
13	1.58 \pm 0.08	1.69 \pm 1.03	2.33 \pm 0.37	2.59 \pm 0.36
14	3.60 \pm 0.88	1.93 \pm 0.20	3.24 \pm 0.28	2.98 \pm 0.21

Table S4. Raw T_1 and NOE values for 75 nm LCBs at 11.7 T and 14.1 T

Carbon Site	11.7 T		14.1 T	
	T_1 (s)	NOE	T_1 (s)	NOE
γ	0.37 \pm 0.04	2.04 \pm 0.23	0.41 \pm 0.03	2.24 \pm 0.04
α	0.26 \pm 0.05	2.22 \pm 0.14	0.34 \pm 0.06	2.41 \pm 0.16
2	0.68 \pm 0.12	1.48 \pm 0.21	0.78 \pm 0.06	1.51 \pm 0.23
4-11	0.64 \pm 0.11	1.87 \pm 0.13	0.76 \pm 0.03	1.96 \pm 0.07
12	0.76 \pm 0.22	1.96 \pm 0.22	0.88 \pm 0.04	2.09 \pm 0.11
13	2.03 \pm 0.97	2.23 \pm 0.08	2.32 \pm 0.13	2.24 \pm 0.26
14	2.38 \pm 2.32	2.47 \pm 0.21	3.66 \pm 0.81	3.17 \pm 0.31

Table S5. Raw T_1 and NOE values for 110 nm LCBs at 11.7 T and 14.1 T

Carbon Site	11.7 T		14.1 T	
	T_1 (s)	NOE	T_1 (s)	NOE
γ	0.47 \pm 0.02	2.79 \pm 0.07	0.55 \pm 0.01	2.62 \pm 0.10
α	0.33 \pm 0.03	2.06 \pm 0.96	0.37 \pm 0.04	2.61 \pm 0.12
2	0.66 \pm 0.10	1.62 \pm 0.08	0.59 \pm 0.08	1.88 \pm 0.23
4-11	0.95 \pm 0.03	2.30 \pm 0.24	0.83 \pm 0.01	2.49 \pm 0.03
12	0.94 \pm 0.07	1.80 \pm 0.66	1.45 \pm 0.28	2.50 \pm 0.30
13	2.16 \pm 0.96	2.79 \pm 0.68	3.33 \pm 0.28	2.60 \pm 0.29
14	3.78 \pm 1.00	3.02 \pm 0.27	2.48 \pm 0.13	2.80 \pm 0.04

Table S6. Raw T_1 and NOE values for 100 nm unilamellar vesicles at 11.7 T and 14.1 T

Carbon Site	11.7 T		14.1 T	
	T_1 (s)	NOE	T_1 (s)	NOE
γ	0.58 \pm 0.01	2.77 \pm 0.01	0.54 \pm 0.00	2.87 \pm 0.04
α	0.38 \pm 0.01	2.35 \pm 0.18	0.40 \pm 0.02	2.77 \pm 0.41
2	0.50 \pm 0.04	2.64 \pm 0.20	0.41 \pm 0.04	1.90 \pm 0.47
4-11	0.79 \pm 0.01	2.45 \pm 0.04	0.81 \pm 0.01	2.30 \pm 0.09
12	1.17 \pm 0.14	2.49 \pm 0.10	1.08 \pm 0.04	1.94 \pm 0.19
13	1.86 \pm 0.10	2.40 \pm 0.09	2.36 \pm 0.22	2.41 \pm 0.18
14	3.16 \pm 0.18	2.77 \pm 0.04	3.17 \pm 0.18	2.86 \pm 0.10