Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Shiga Toxin Binding Alters Lipid Packing and Domain Structure of Gb_3-Containing Membranes: A Solid-State NMR Study

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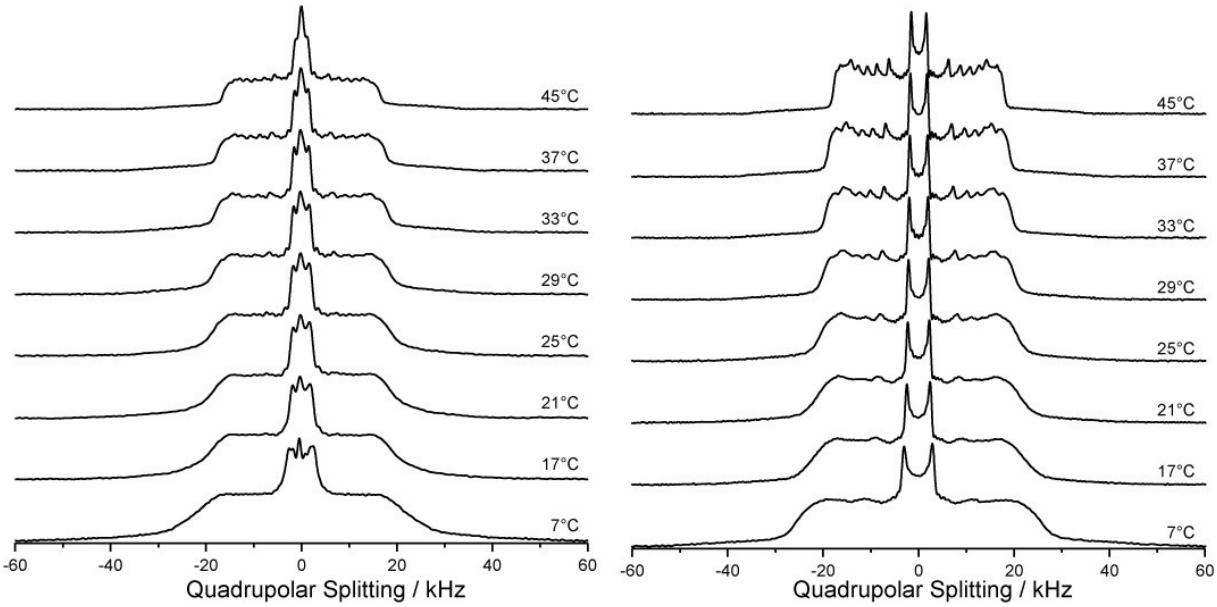
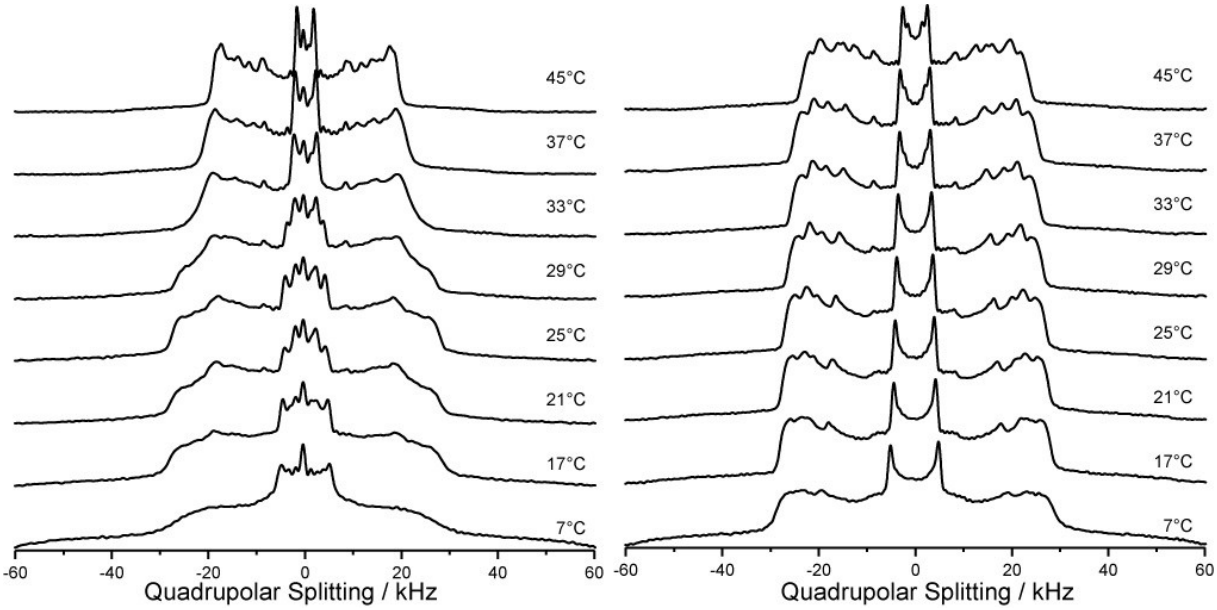
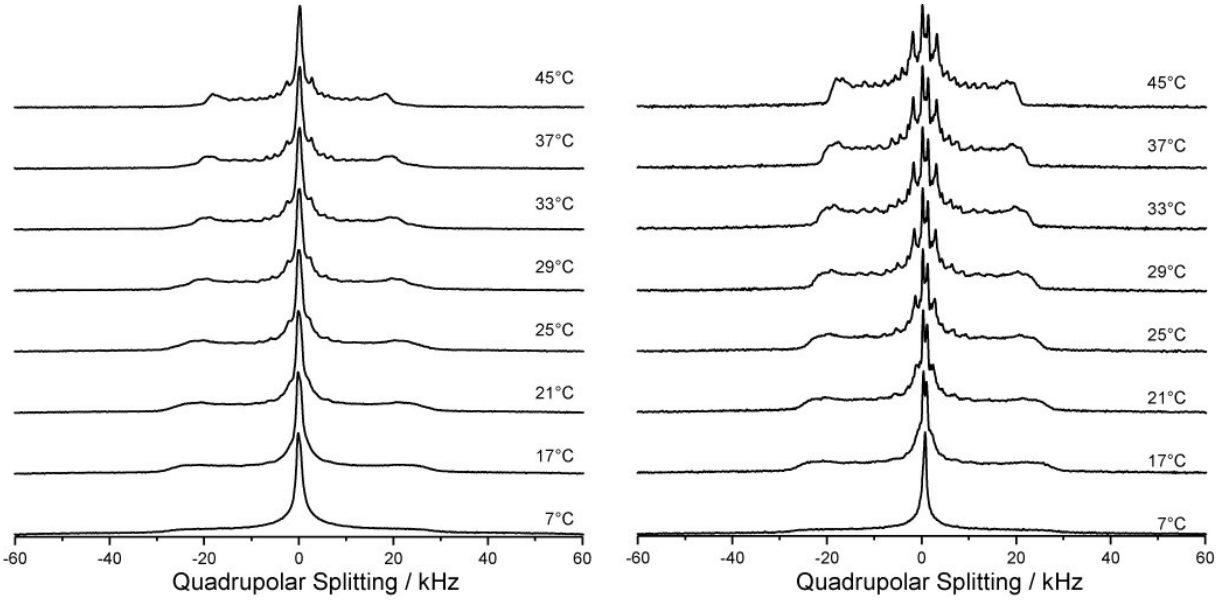


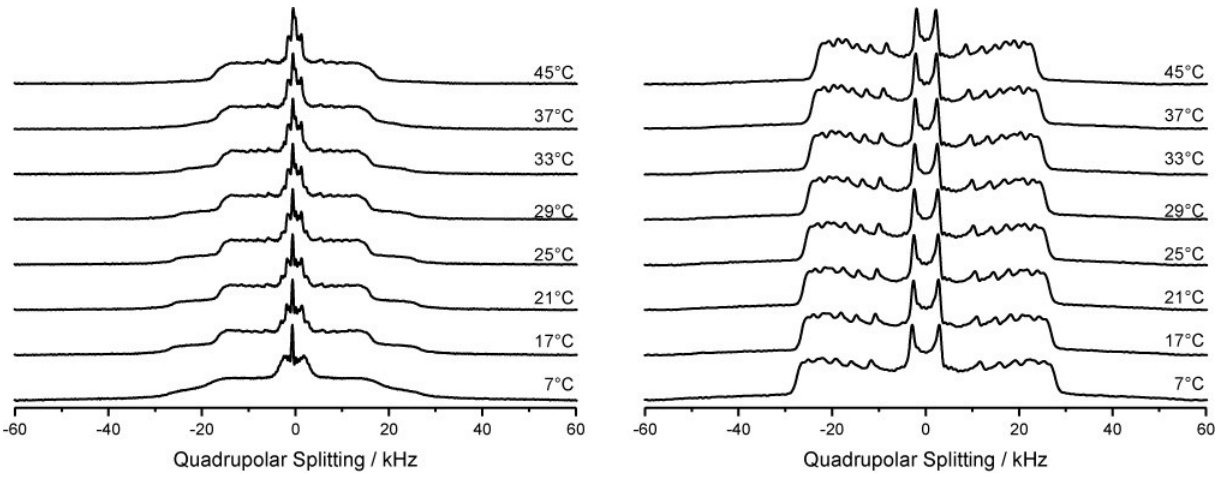
Supplementary Figure S1. ^{2}H NMR spectra for the deuterated POPC-d_{31} of the quaternary lipid mixture lignoceryl-Gb_3/POPC-d_{31}/PSM/cholesterol (molar ratio: 5:40:35:20) in the presence of STxB (molar protein to lipid ratio of 1:120, left) and in the absence of STxB (right) at the given temperatures.



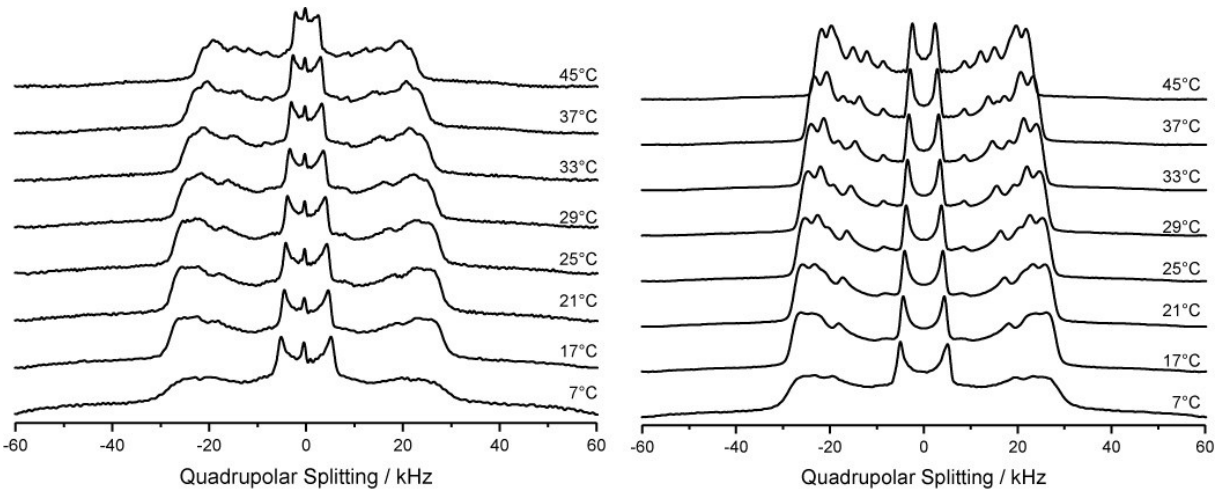
Supplementary Figure S2. ^{2}H NMR spectra for the deuterated PSM-d_{31} of the quaternary lipid mixture lignoceryl-Gb_3/POPC/PSM-d_{31}/cholesterol (molar ratio: 5:40:35:20) in the presence of STxB (molar protein to lipid ratio of 1:120, left) and in the absence of STxB (right) at the given temperatures.



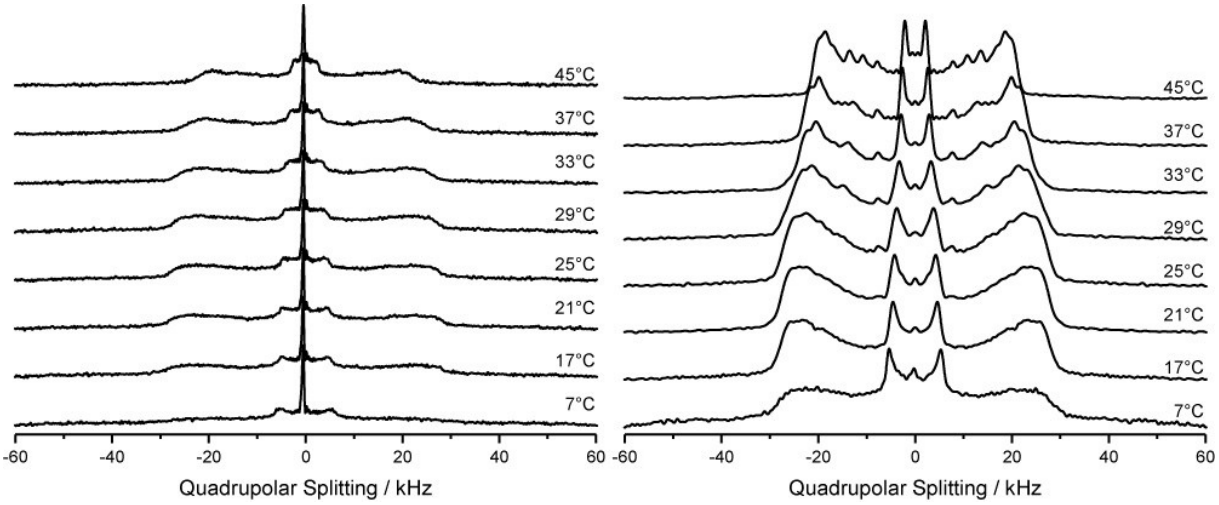
Supplementary Figure S3. ^{2}H NMR spectra for the deuterated lignoceryl-Gb_3-d_{47} of the quaternary lipid mixture lignoceryl-Gb_3-d_{47}/POPC/PSM /cholesterol (molar ratio: 5:40:35:20) in the presence of STxB (molar protein to lipid ratio of 1:120, left) and in the absence of STxB (right) at the given temperatures.



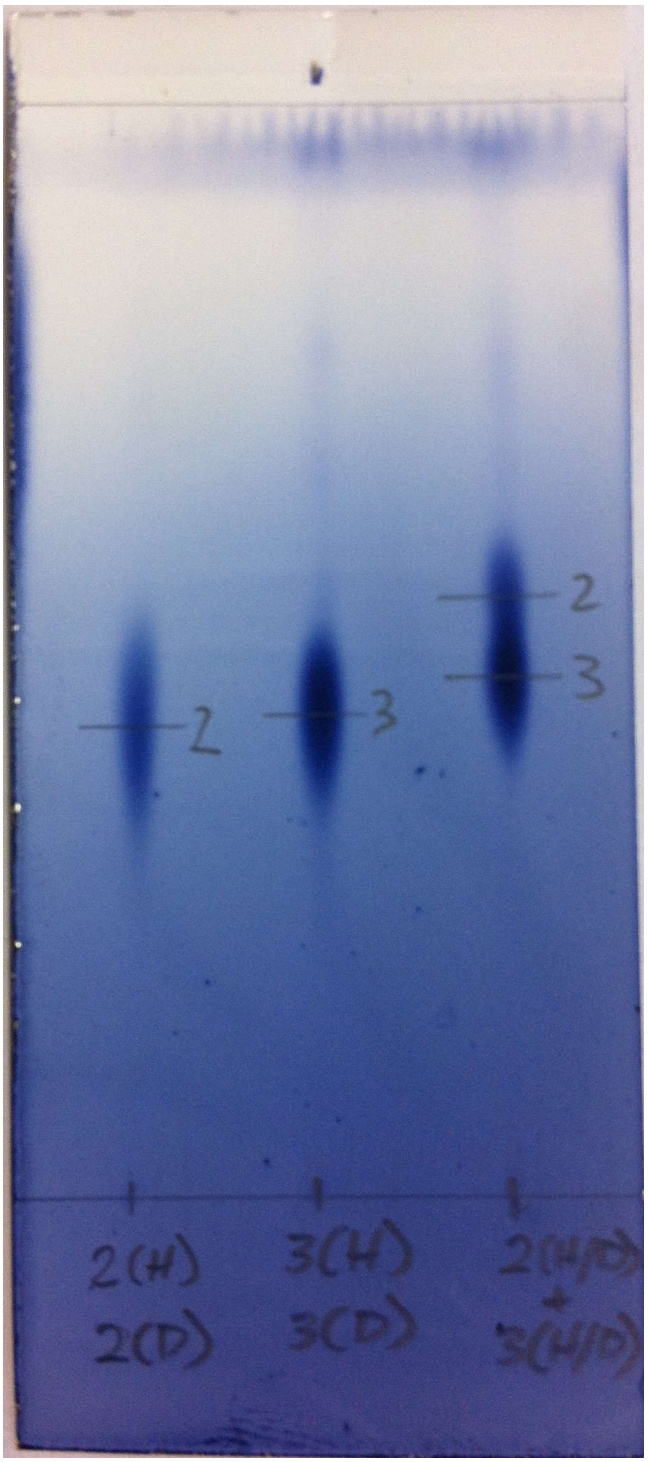
Supplementary Figure S4. ^{2}H NMR spectra for the deuterated POPC-d_{31} of the quaternary lipid mixture palmitoyl-Gb_3/POPC-d_{31}/PSM/cholesterol (molar ratio: 5:40:35:20) in the presence of STxB (molar protein to lipid ratio of 1:120, left) and in the absence of STxB (right) at the given temperatures.



Supplementary Figure S5. ^{2}H NMR spectra for the deuterated PSM-d_{31} of the quaternary lipid mixture palmitoyl-Gb_3/POPC/PSM-d_{31}/cholesterol (molar ratio: 5:40:35:20) in the presence of STxB (molar protein to lipid ratio of 1:120, left) and in the absence of STxB (right) at the given temperatures.



Supplementary Figure S6. ^{2}H NMR spectra for the deuterated palmitoyl-Gb_3-d_{31} of the quaternary lipid mixture palmitoyl-Gb_3-d_{31}/POPC/PSM/cholesterol (molar ratio: 5:40:35:20) in the presence of STxB (molar protein to lipid ratio of 1:120, left) and in the absence of STxB (right) at the given temperatures.



Supplementary Figure S7. Thin layer chromatogram of all Gb_3 lipids used in this study. The plate was developed using H_2O, CH_3OH and CH_2Cl_2 (1, 30, 100, v/v/v). After the end of the chromatographic run and careful drying the different compounds were rendered visible by spraying with cerium (IV)/ammonium molybdate solution.

Supplementary Table S1: Calculated chain extent L_c* in Å for the respective deuterated lipid in lignoceryl-Gb_3 /POPC/PSM /cholesterol (5:40:35:20 mol/mol/mol/mol) membranes. The experimental error of the L_c* calculation is ~0.2 Å for Gb_3 and ~0.1 for POPC or PSM.

Temperature	Gb_3-d_{47}		POPC-d_{31}		PSM-d_{31}	
/°C		+Shiga		+Shiga		+Shiga
25	21.0	21.0	14.1	13.5	15.8	15.4
37	19.5	18.9	13.6	13.1	15.4	14.6
45	18.9	18.5	13.3	13.0	14.9	14.1

Supplementary Table S2: Mean order parameter for the respective deuterated lipid in lignoceryl-Gb_3-d_{47}/POPC/PSM /cholesterol (5:40:35:20 mol/mol/mol/mol) membranes. The typical experimental error on the average order parameter is <0.01.

Temperature	Gb_3-d_{47}		POPC-d_{31}		PSM-d_{31}	
/°C		+Shiga		+Shiga		+Shiga
25	0.26	0.27	0.26	0.23	0.35	0.33
37	0.21	0.21	0.23	0.21	0.33	0.28
45	0.20	0.19	0.22	0.21	0.30	0.26

Supplementary Table S3: Calculated chain extent L_c* in Å for the respective deuterated lipid in palmitoyl-Gb_3/POPC/PSM/cholesterol (5:40:35:20 mol/mol/mol/mol) membranes. The experimental error of the L_c* calculation is ~0.2 Å for Gb_3 and ~0.1 for POPC or PSM.

Temperature	Gb_3-d_{31}		POPC-d_{31}		PSM-d_{31}	
/°C		+Shiga		+Shiga		+Shiga
25	16.4	15.6	15.4	12.8	16.2	16.3
37	15.3	15.1	15.0	12.9	15.6	15.6
45	14.6	15.0	14.9	12.9	15.2	14.9

Supplementary Table S4: Mean order parameter for the respective deuterated lipid in palmitoyl-Gb_3/POPC/PSM/cholesterol (5:40:35:20 mol/mol/mol/mol) membranes. The typical experimental error on the average order parameter is <0.01.

Temperature /°C	Gb_3-d_{31}	+Shiga	POPC-d_{31}	+Shiga	PSM-d_{31}	+Shiga
25	0.39	0.35	0.33	0.20	0.38	0.39
37	0.32	0.31	0.31	0.20	0.34	0.34
45	0.28	0.29	0.30	0.20	0.31	0.30