Supplementary Materials

Effect of Shiga toxin on inhomogeneous biological membrane structure determined by small-angle scattering

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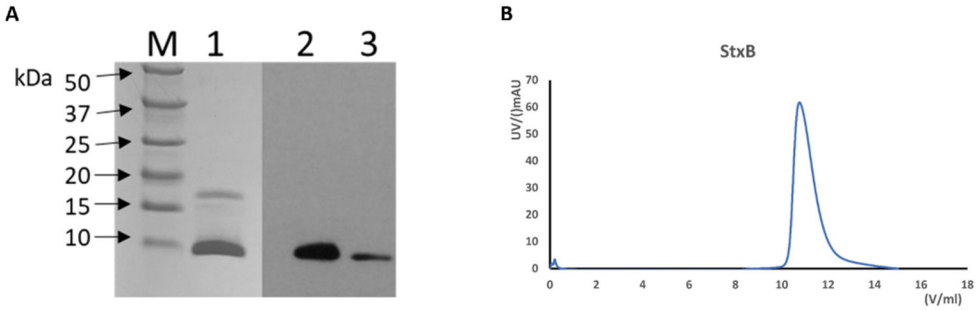

Figure S1. Characterization of the purified Shiga toxin B-subunit. A) Tricine-SAS-PAGE (Lanes M-1) and Western-blot analysis (Lanes 2-3) of cytoplastic extracts of E. coli BL21 (DE3) ; B) FPLC profile of Shiga toxin B-subunit.

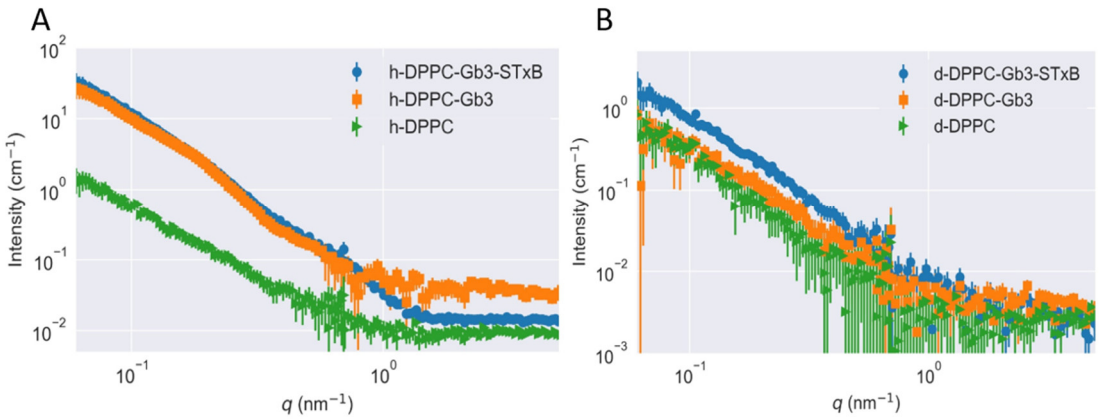

Figure S2. Small-angle scattering curves of the SUV samples of Gb3 and DPPC mixture ([Gb3]/[DPPC] = 0.1/1 illustrated with error bar. Measurements were performed at T = 25°C. (A) small-angle neutron scattering curves of [h-DPPC]/[d-DPPC] = 1/0; (B) small-angle neutron scattering curves of [h-DPPC]/[d-DPPC] = 0/1.

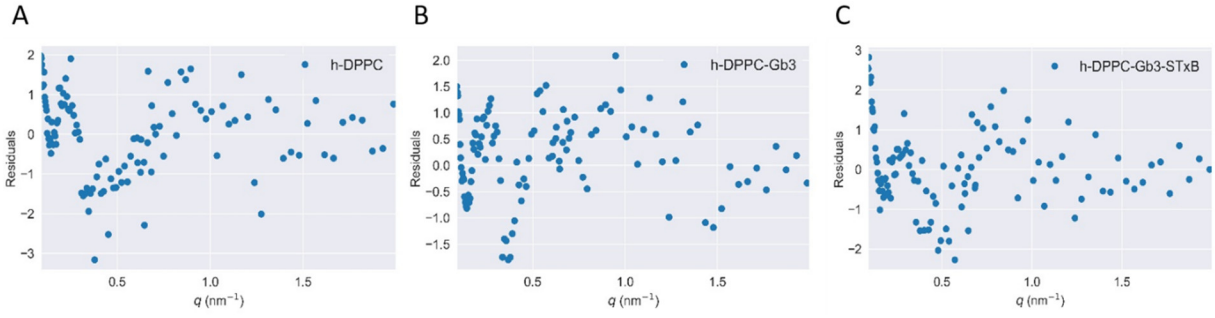

Figure S3. Fitting residuals of scattering for the [h-DPPC]/[d-DPPC] = 1/0 SUV sample using polydisperse three-shell model. The SUV were prepared as [Gb3]/[DPPC] = 0.1/1. Measurements were performed at T = 25°C. A) Empty DPPC vesicle; B) Gb3 reconstructed DPPC vesicle; C) Shiga toxin B subunit incubated with Gb3 reconstructed DPPC vesicle.

Table S1. The overall size parameters of [h-DPPC]/[d-DPPC] = 0/1 SUV vesicle ([Gb3]/[DPPC] = 0.1/1, 1% w/v DPPC in D2O, pH 7.0). Measured by dynamic light scattering.

	DPPC (nm)	DPPC-Gb3 (nm)	DPPC-Gb3-STxB (nm)
R1	66.5	71.5	69.9
R2	69.7	67.9	64.1
R3	76.2	75.2	63.7
Average	70.8	71.5	65.9

Table S2. The fitting parameters for scattering data used in model membranes. The reduced chi-square value is listed to prove the fitting fidelity.

	Fitting interval (nm^{-1})	**Thickness of head-group (nm)**	**Thickness of tail (nm)**	**Lognormal distribution**		**Reduced Chi-square**
				R_{med} (nm) fixed	σ fixed	
h-DPPC	0.09-2	3.33(5)	0.80(8)	18	0.5	1.1
h-DPPC-Gb3	0.09-2	3.10(13)	0.85(7)	18	0.5	0.7
h-DPPC-Gb3-STxB	0.09-2	2.50(15)	1.13(8)	18	0.5	1.1

Table S3. The fitting parameters for scattering data used in Gb3 microdomains by the model-independent Guinier law for elongated objects with the assumption that the microdomains form elongated aggregates.

	Fitting interval (nm^{-1})	**R_g (nm)**	**I_0 (a.u.)**
h-DPPC-Gb3-STxB	0.06~0.15	7.8(7)	0.034(3)
h-DPPC-Gb3	0.06~0.20	5.3(7)	0.011(1)