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Supplemental Information

Membrane Adhesion via Glycolipids Occurs for Abundant Saccharide Chemistries

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Supporting Information

1.) Electrostatic repulsion between charged surfaces in a monovalent electrolyte

For weakly charged surfaces in a monovalent electrolyte the pressure Π_{el} associated with the electrostatic repulsion is given as [1]:

$$\Pi_{el}(d_w) \cong 2k_BT\rho_0[\cosh(e\psi_m(d_w)/k_BT) - 1],$$

where ρ_0 is the number density of monovalent ions in the bulk, e is the electron charge, and ψ_m is the electric potential at the midplane (i.e., the center of the water layer). For sufficiently low charge densities (i.e., in the Debye-Hückel limit) and within the weak-overlap approximation, ψ_m is proportional to the surface electric potential ψ_0:

$$\psi_m(d_w) = 2\psi_0 e^{-\kappa d_w/2},$$

where

$$\kappa^{-1} = \sqrt{\frac{\varepsilon_0 \varepsilon k_B T}{2e^2 \rho_0}}$$

is the Debye length and ψ_0 follows from the surface charge density σ according to the relation

$$\sigma^2 = 2\varepsilon\varepsilon_0 k_B T \sum_j \rho_0 \left[\exp\left(-z_j e\psi_0/k_BT\right) - 1\right],$$

where $z_j = \pm 1$ is the charge number of the cations and anions, respectively.

2.) Lamellar periodicities obtained by SAXS for of DMPC membranes containing *Psyc-sat* and DMPG

Fig. S1 shows $d(f_{gly})$ for DMPC membranes loaded with *Psyc-sat*, a glycolipid with a mono-galactose headgroup. The lamellar periodicity decreases approximately linearly with increasing f_{gly}. The smallest value is $d \approx 6$ nm at $f_{gly} = 0.2$.

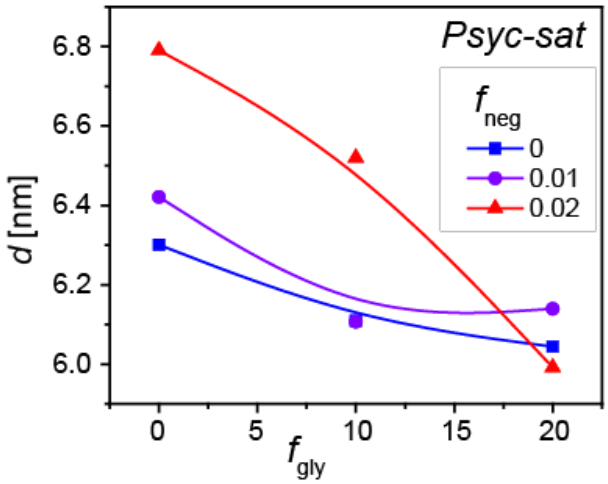

Figure S1: Lamellar periodicities *d* obtained by SAXS for DMPC lipid membrane multilayers containing various fractions f_{gly} of *Psyc-sat* and f_{neg} of the negatively charged lipid DMPG. The measurements were conducted at 50 °C. Solid lines are guides to the eye.

3.) Neutron diffraction (ND) measurements under bulk water conditions

The results of ND measurements of POPC membranes loaded with *DGDG-unsat* at $f_{gly} = 0.2$ and $f_{neg} = 0$, and of DMPC membranes loaded with *LacCer-sat* at $f_{gly} = 0.2$ and $f_{neg} = 0$ under bulk water conditions are summarized in Fig. S2. The intensities of the second Bragg sheets were found to be too weak to be analyzed.

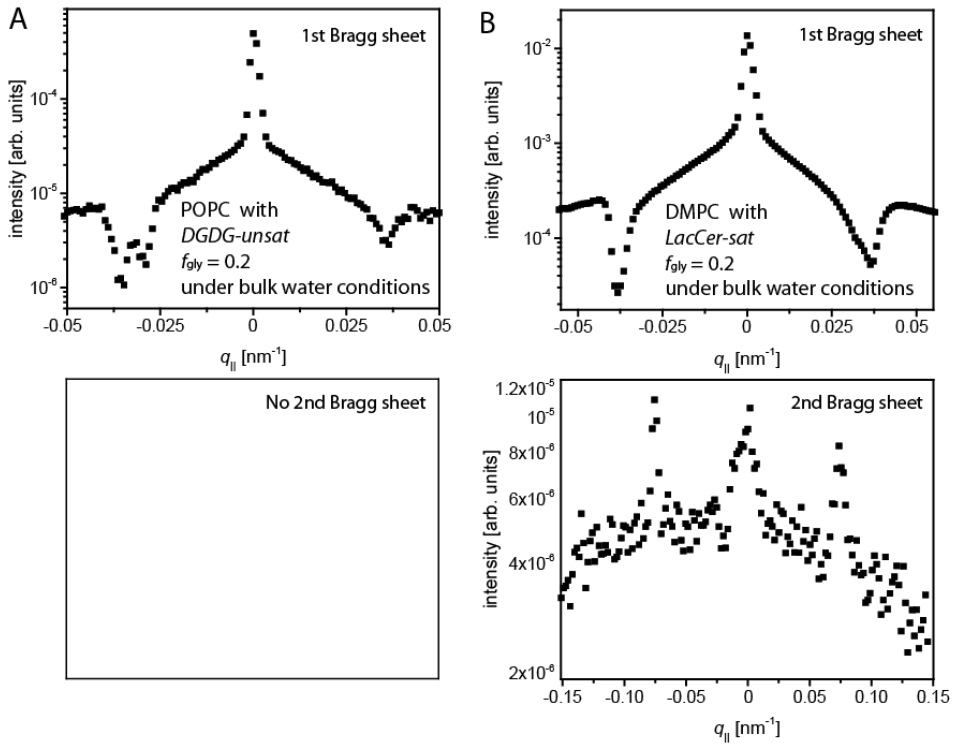

Figure S2: Intensities of the first (top) and second (bottom) Bragg sheets of (A) POPC membranes loaded with *DGDG-unsat* at $f_{gly} = 0.2$ and $f_{neg} = 0$ and (B) DMPC membranes loaded with *LacCer-sat* at $f_{gly} = 0.2$ and $f_{neg} = 0$, both under bulk water conditions.

4.) Accounting for absorption of the neutron beam in the modeled Bragg sheets

Close to the conditions $\Omega = O$ and $\Omega = \Gamma$ the incident and scattered neutron beams, respectively, travel essentially parallel to the sample plane and thus get strongly absorbed on the way through the sample. While crystalline silicon is practically transparent to neutrons on the length scales relevant for the present work, beam absorption through incoherent scattering by the lipid layer is considerable, because the lipids are hydrogenous, i.e., they contain light hydrogen (^1H). The attenuation coefficient for DMPC (chemical formula: $C_{36}H_{72}NO_8P$) at a mass density of 1 g cm^{-3} is $\mu \approx 5$ cm^{-1} at $\lambda = 4.518$ Å [2]. Hydrating D_2O has negligible contribution to absorption.

The average thickness of the lipid film on the silicon wafer is $h \approx 1$ µm, as follows from the deposited lipid amount (≈ 1 mg), their mass density (≈ 1 g cm^{-3}), as well as from the approximate extensions of the coated region in the direction parallel to the beam ($L_{||} \approx 2$ cm) and in the perpendicular direction ($L_{\perp} \approx 5$ cm). For each coated surface element along the direction of the beam ($0 \leq x \leq L_{||}$), the maximal path length is $s_{max}^{in}(x) = x$ for the incident beam and $s_{max}^{sc}(x) = L_{||} - x$ for the scattered beam. Depending on the angle of incidence, the actual path length is given as

$s_{in}(\Omega, x) = MIN\left(\left[s_{max}^{in}(x);\ h/\sin(|\Omega|)\right]\right)$ for the incident beam

and

$s_{sc}(\Omega, x) = MIN([s_{max}^{sc}(x);\ h/\sin(|\Omega - \Gamma|)])$ for the scattered beam

The overall attenuation by the sample on the way to the detector, represented as the transmission function $T(\Omega)$ thus follows as $T(\Omega) = T_{in}(\Omega) \cdot T_{sc}(\Omega)$, where

$$T_{in}(\Omega) = \frac{1}{L_{||}} \int_0^{L_{||}} e^{-\mu \cdot s_{in}(\Omega, x)} dx$$

$$T_{sc}(\Omega) = \frac{1}{L_{||}} \int_0^{L_{||}} e^{-\mu \cdot s_{sc}(\Omega, x)} dx$$

5.) Influence of negatively charged phospholipids in the interaction of phospholipid bilayers containing *TetraG-sat*

Fig. S3 shows $d(f_{gly})$ for DPPC membranes loaded with *TetraG-sat*, a glycolipid with a linear tetrasaccharide headgroup composed of (galactose)-(N-acetyl-galactose)-(galactose)-(glucose). There is a strong increase of d with f_{gly}., which is steep in the beginning until it reaches saturation. Incorporation of negatively charged lipids has no pronounced effect in the investigated range ($f_{neg} \leq 0.05$)

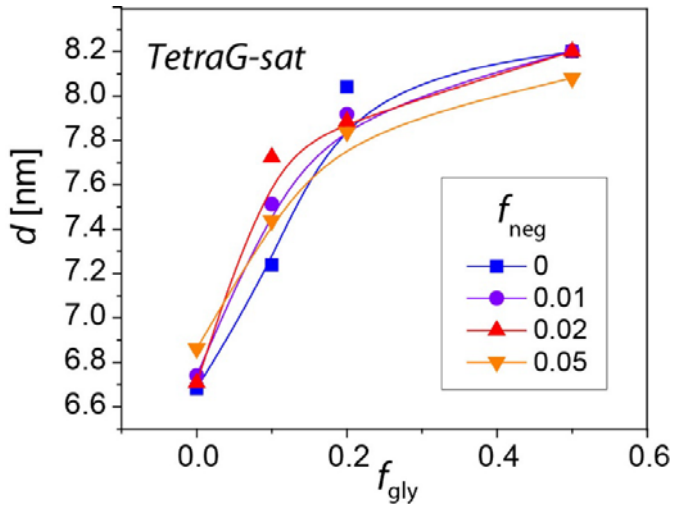

Figure S3: Lamellar periodicities d obtained by SAXS for DPPC lipid membrane multilayers containing various fractions f_{gly} of *TetraG-sat* and f_{neg} of the negatively charged lipid DPPG. The measurements were conducted at 50 °C. Solid lines are guides to the eye.

References

[1] Israelachvili, J. N., *Intermolecular and surface forces*. Academic press: 2011

[2] NIST Center for Neutron Research, https://www.ncnr.nist.gov/resources/activation/