Electronic Supplementary Material (ESI) for Soft Matter.

Interplay of Membrane Fluidity, Acyl Chain Order and Area per Lipid on Partitioning of Two Antidepressants Paroxetine and Sertraline

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Supplementary Information

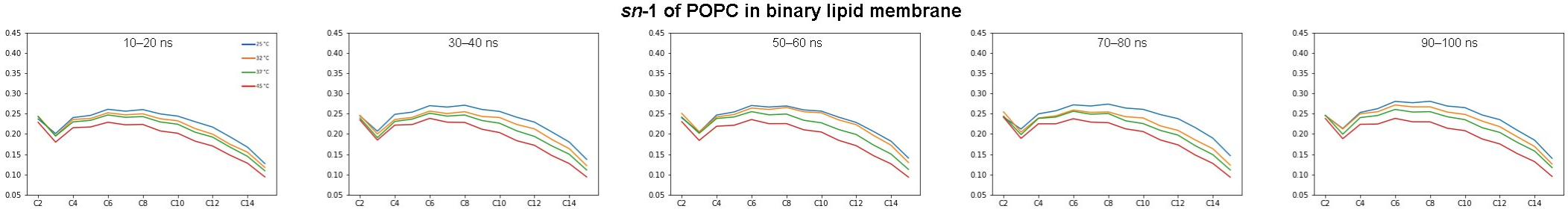

Figure S1. The S_{CD} of the POPC *sn*-1 chain in the binary lipid membrane at (ns) at varying temperatures: 25, 32, 37, and 45 °C at intermittent intervals along the simulation. The system is shown to be stable in the last 50 ns of the simulation; thus, it is reasonable to use the last 50 ns for the calculation of the acyl chain order parameters.

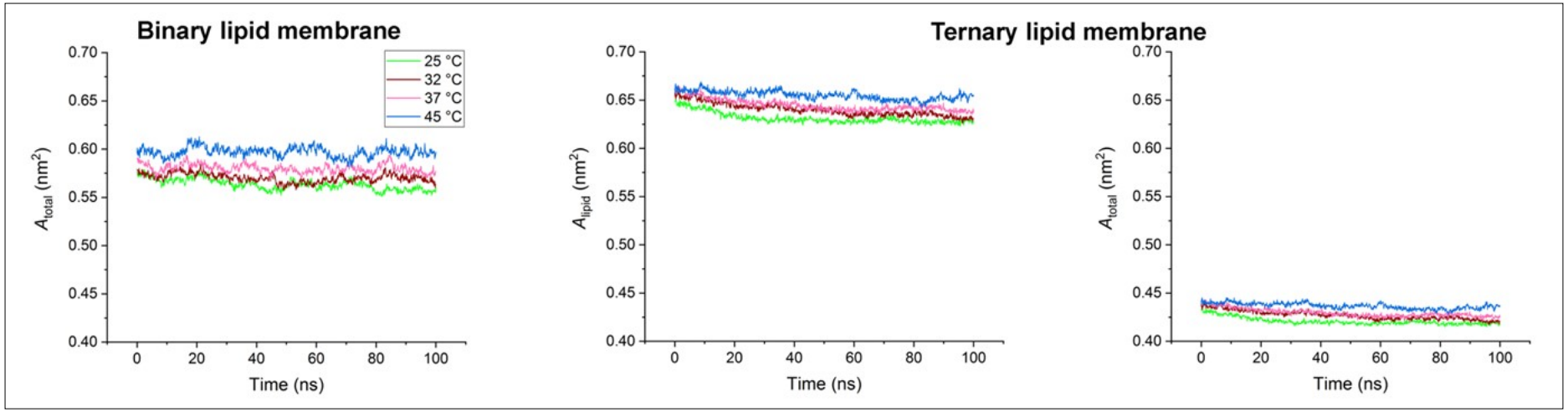

Figure S2. The A_{total} (nm^2) of the binary lipid membrane (top) and the A_{total} and A_{lipid} (nm^2) of the ternary lipid membrane (bottom) plotted as a function of the simulation time (ns) at varying temperatures: 25, 32, 37, and 45 °C.

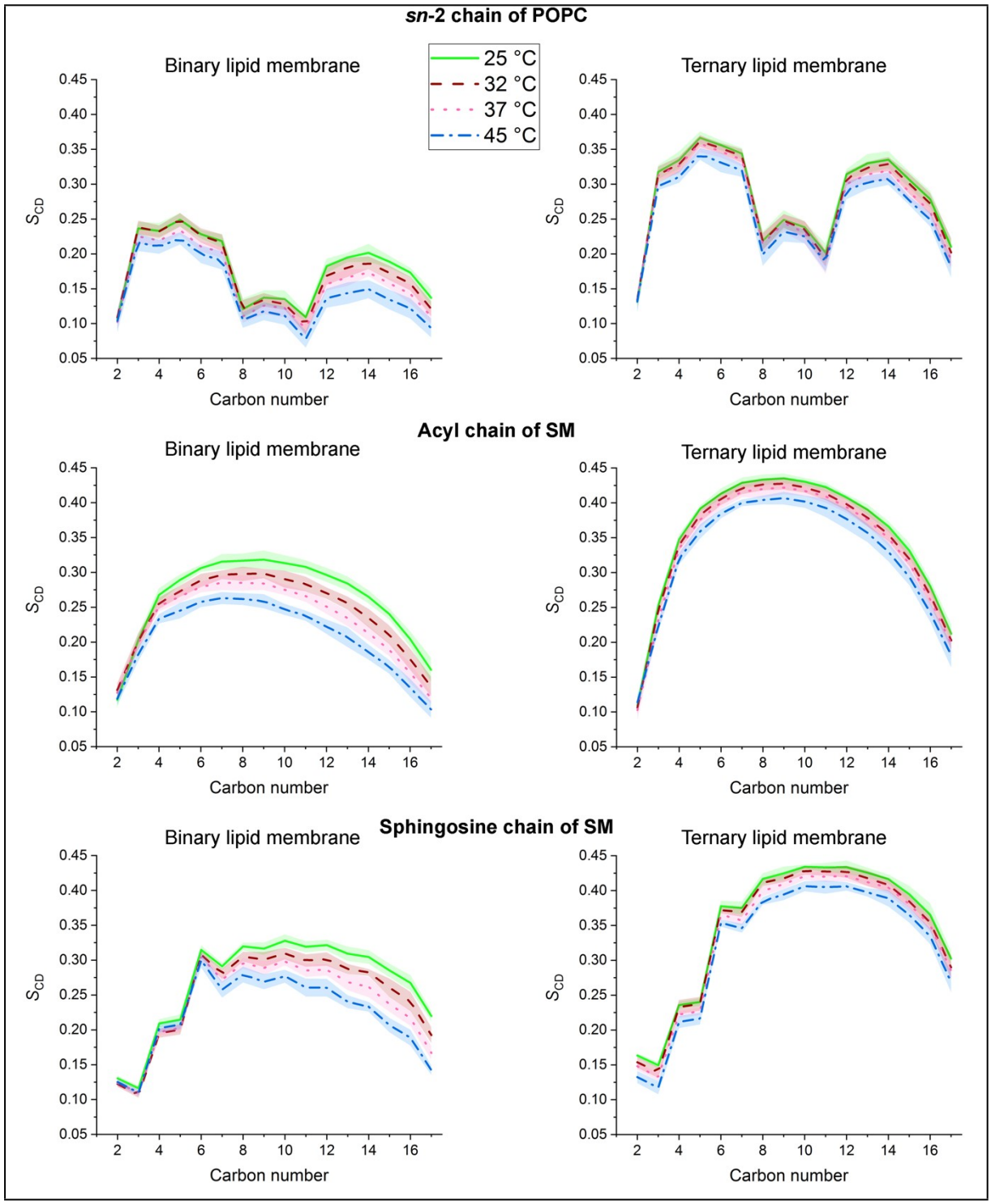

Figure S3. The order parameter vs. the carbon number for the *sn*-2 chain of POPC, the acyl and sphingosine chains of SM in the POPC:SM (left) and POPC:SM:Chol (right) lipid membranes at varying temperatures: 25, 32, 37, and 45 °C.

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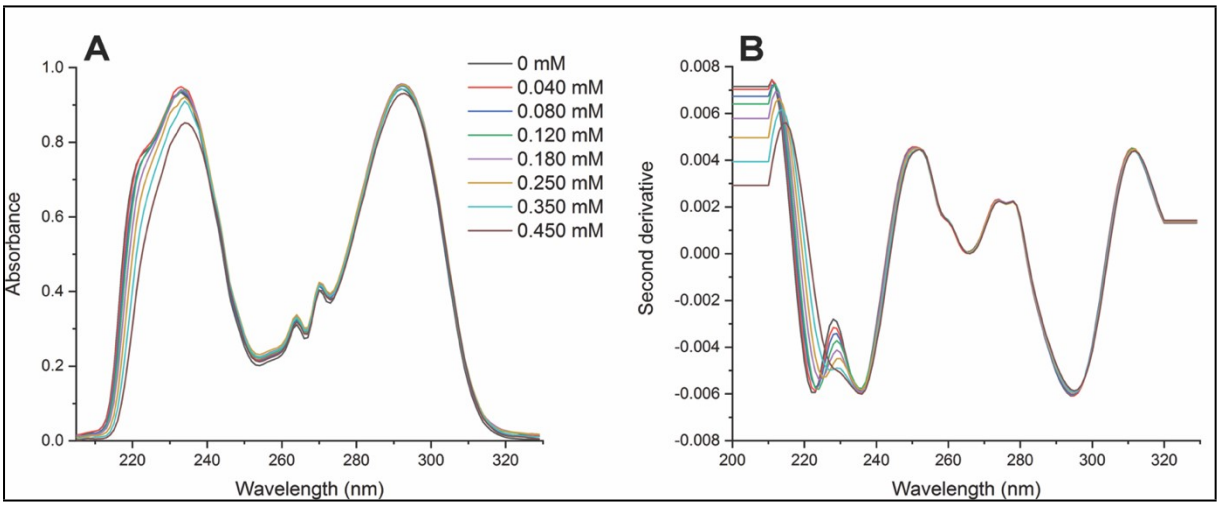

Figure S4. (A) Absorption spectra and (B) second derivative spectra of PAX in HEPES (pH 7.4, 25 °C) consisting of distinct concentrations of POPC:SM LUVs (mM): (1) 0; (2) 0.040; (3) 0.080; (4) 0.120; (5) 0.180; (6) 0.250; (7) 0.350; (8) 0.450.

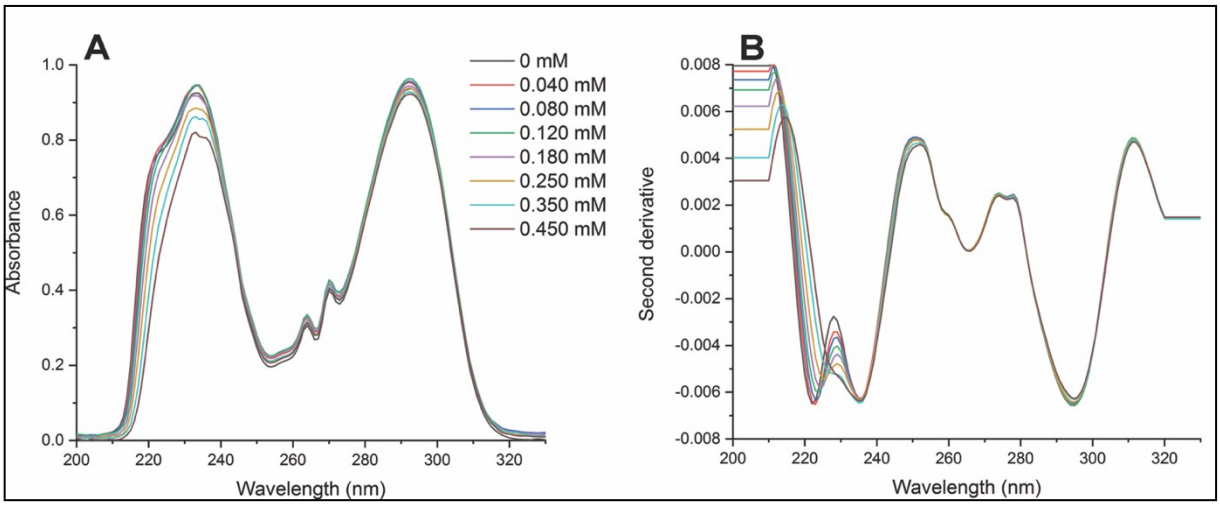

Figure S5. (A) Absorption spectra and (B) second derivative spectra of PAX in HEPES (pH 7.4, 25 °C) consisting of distinct concentrations of POPC:SM:Chol LUVs (mM): (1) 0; (2) 0.040; (3) 0.080; (4) 0.120; (5) 0.180; (6) 0.250; (7) 0.350; (8) 0.450.

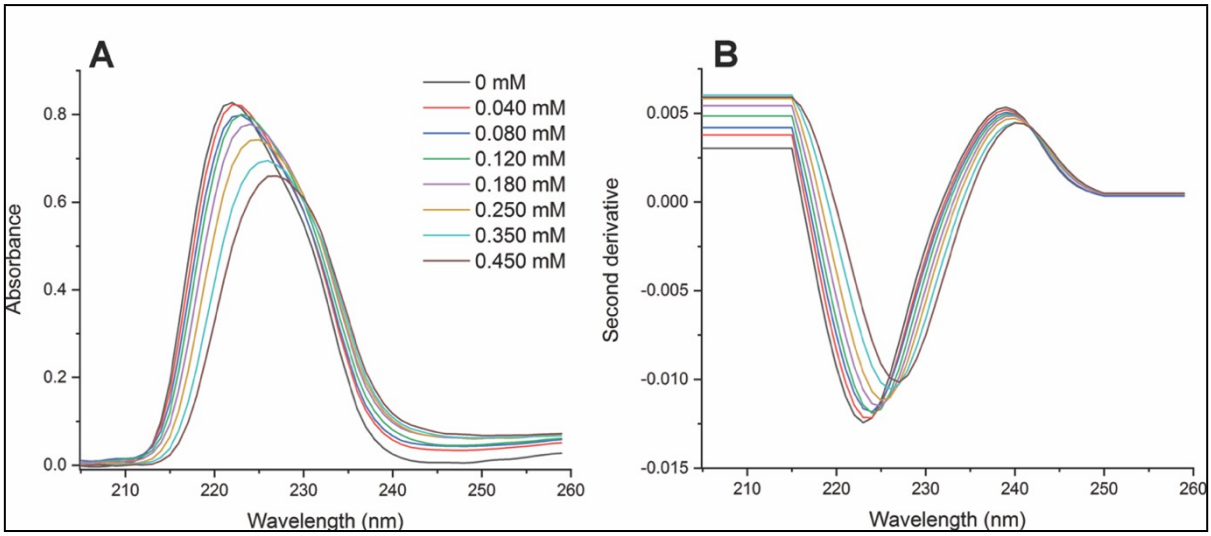

Figure S6. (A) Absorption spectra and (B) second derivative spectra of SER in HEPES (pH 7.4, 25 °C) consisting of distinct concentrations of POPC:SM LUVs (mM): (1) 0; (2) 0.040; (3) 0.080; (4) 0.120; (5) 0.180; (6) 0.250; (7) 0.350; (8) 0.450.

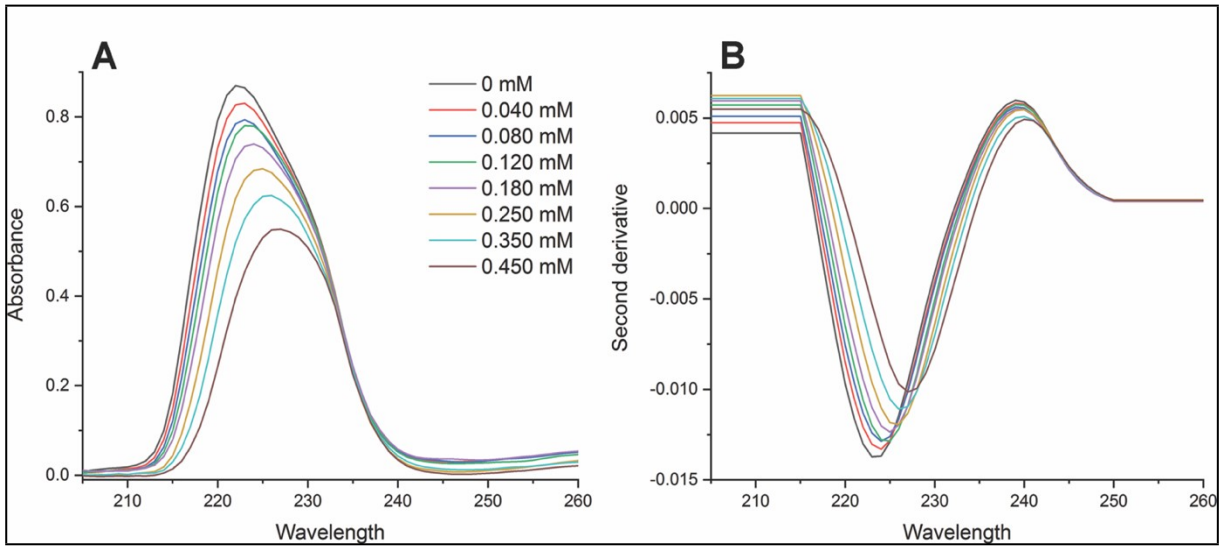

Figure S7. (A) Absorption spectra and (B) second derivative spectra of SER in HEPES (pH 7.4, 25 °C) consisting of distinct concentrations of POPC:SM:Chol LUVs (mM): (1) 0; (2) 0.040; (3) 0.080; (4) 0.120; (5) 0.180; (6) 0.250; (7) 0.350; (8) 0.450.

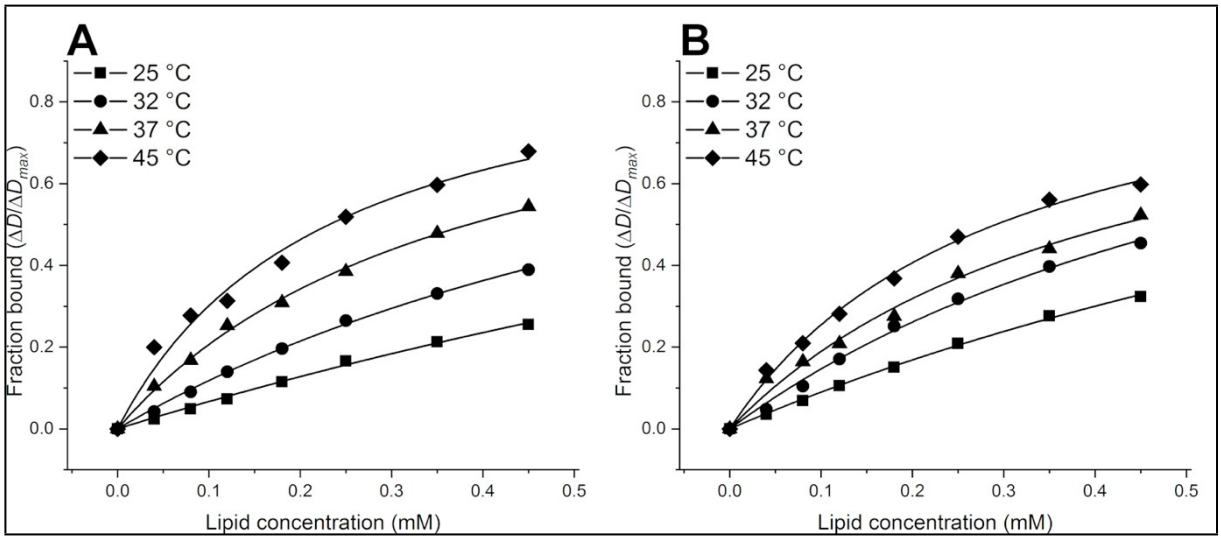

Figure S8. Fraction bound ($\Delta D/\Delta D_{max}$) of PAX in (A) POPC:SM and (B) POPC:SM:Chol LUVs at varied temperatures: 25 °C (filled squares), 32 °C (filled circles), 37 °C (filled triangles) and 45 °C (filled diamonds) versus lipid concentration (mM)

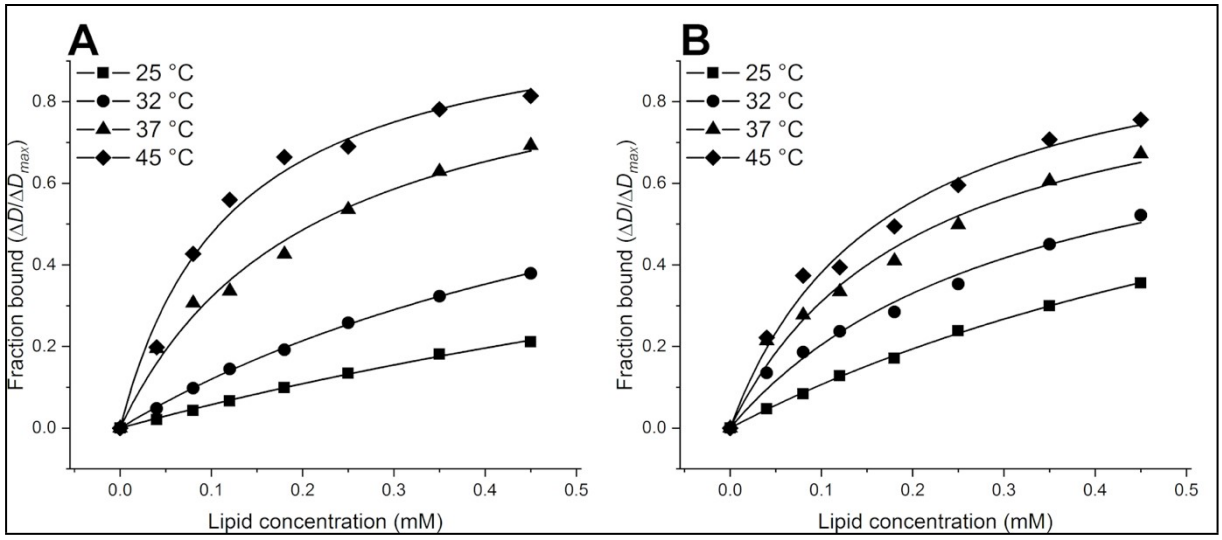

Figure S9. Fraction bound ($\Delta D/\Delta D_{max}$) of SER in (A) POPC:SM and (B) POPC:SM:Chol LUVs at varied temperatures: 25 °C (filled squares), 32 °C (filled circles), 37 °C (filled triangles) and 45 °C (filled diamonds) versus lipid concentration.

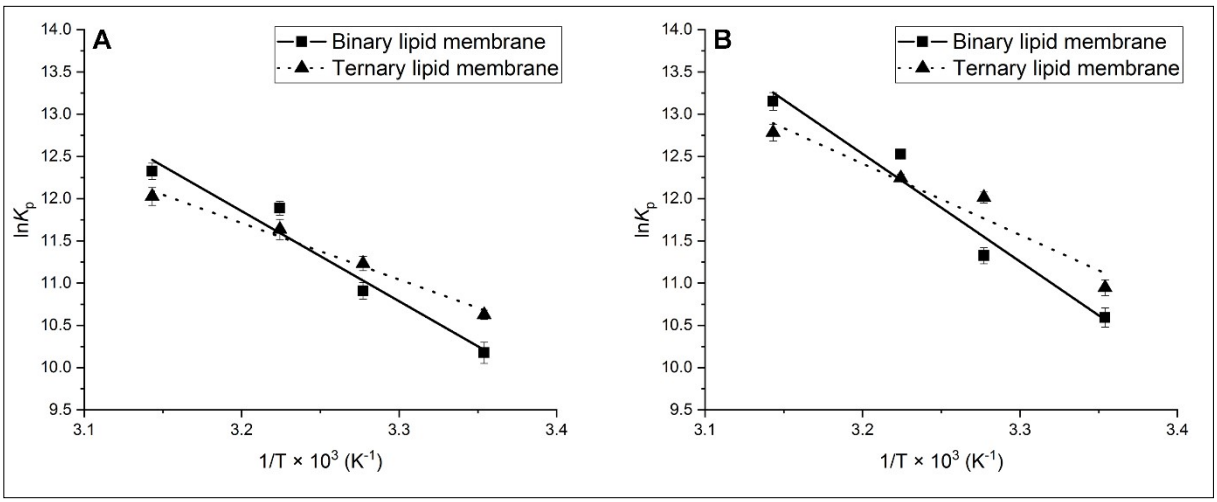

Figure S10. Van't Hoff plots of PAX (A) and SER (B) partitioning into lipid membranes composed of POPC:SM (filled squares) and POPC:SM:Chol (filled triangles).