Supplementary Material

Global SAXS data analysis for multilamellar vesicles: The evolution of the scattering density profile (SDP) model

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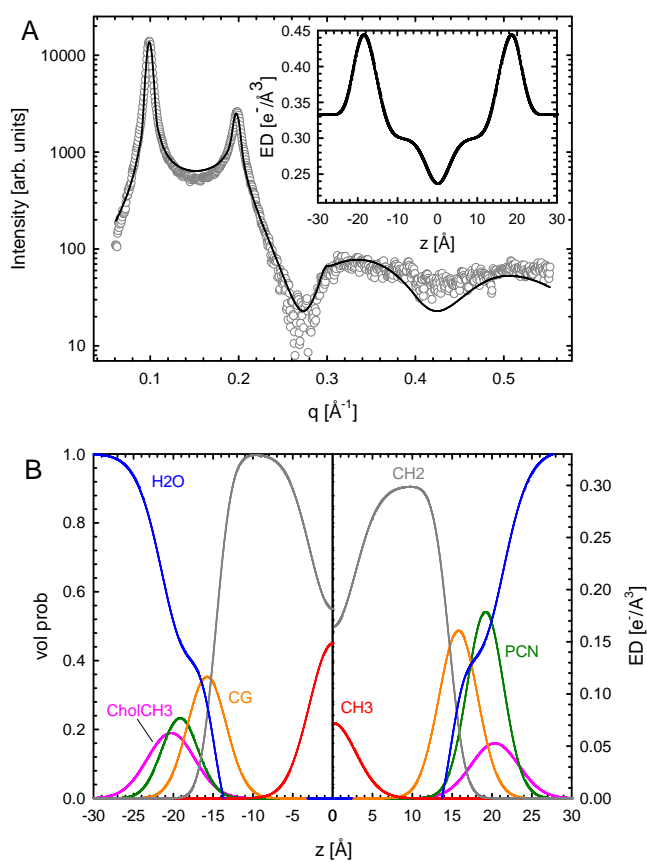
Figure S1: SDP-GAP analysis of DOPC MLVs at 30 °C. Panel A compares the best SDP-GAP fit (black line) to experimental data (grey circles). The insert represents the corresponding electron density profile. Panel B shows the volume probability distribution (left hand side) and the electron density distributions of the considered quasi-molecular fragments (right hand side).

Figure S2: SDP-GAP analysis of DPPC MLVs at 50 °C. Panel A compares the best SDP-GAP fit (black line) to experimental data (grey circles). The insert represents the corresponding electron density profiles. Panel B shows the volume probability distribution (left hand side) and the electron density distributions of the considered quasi-molecular fragments (right hand side).
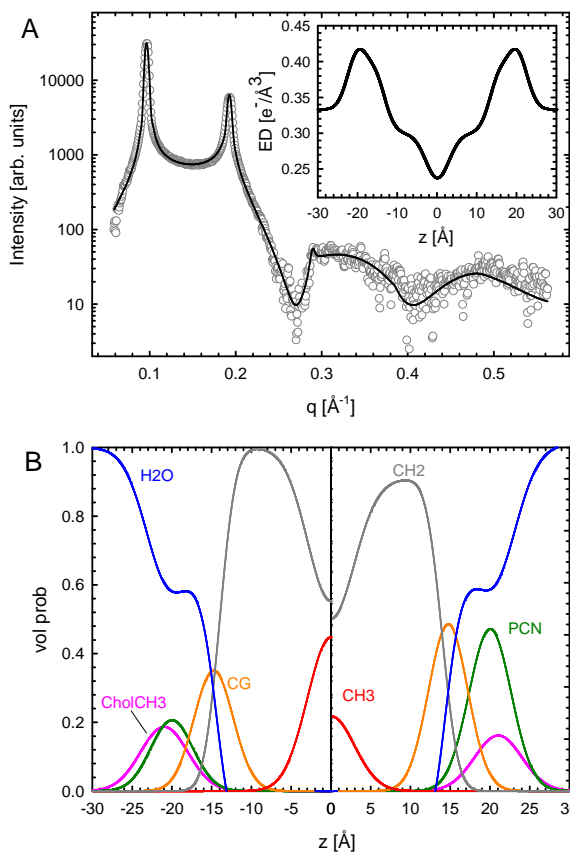

Figure S3: SDP-GAP analysis of POPC MLVs at 30 °C. Panel A compares the best SDP-GAP fit (black line) to experimental data (grey circles). The insert represents the corresponding electron density profiles. Panel B shows the volume probability distribution (left hand side) and the electron density distributions of the considered quasi-molecular fragments (right hand side).
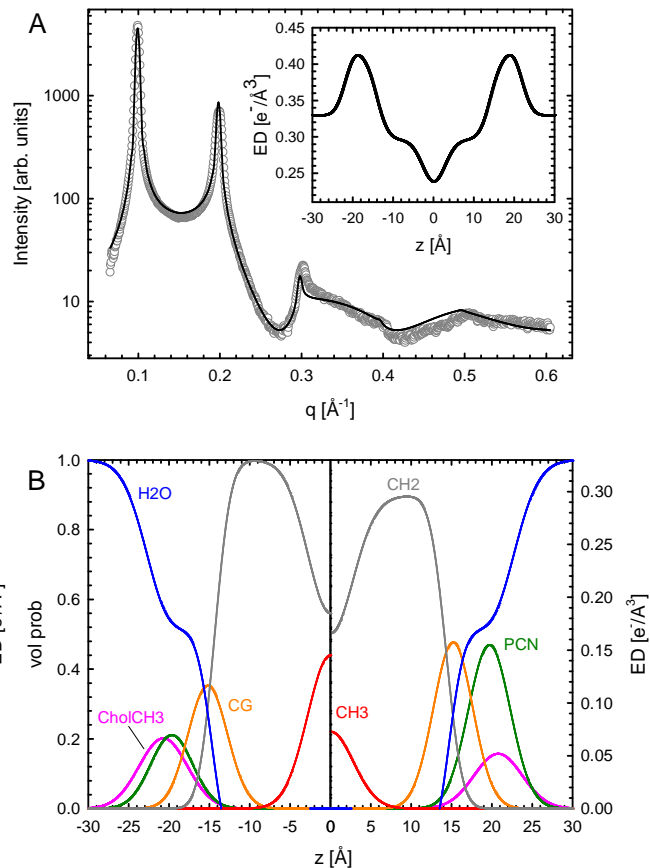
Table S1: Structural parameters of four different phospholipid bilayers analyzed by SDP-GAP. Parameter uncertainties are estimated to be < 2% as described in Materials and Methods.

Par	DPPC	POPC	SOPC	DOPC
Temp	50℃	30℃	30℃	30℃
V_L [Å^3]	1229	1256	1309	1303
V_{HL} [Å^3]	331	331	331	331
A [Å^2]	63.1	65.4	66.3	67.6
d_B [Å]	39	38.4	39.5	38.5
d_{HH} [Å]	37.9	37.3	38.7	36.9
d_C [Å]	13.9	14.0	14.6	14.2
$z_{CholCH3}{}^{*}$ [Å]	21.2	20.7	21.2	20.3
$\sigma_{CholCH3}{}^{\dagger}$ [Å]	2.98	2.98	2.98	2.98
$z_{PCN}{}^{*}$ [Å]	20.2	19.7	20.2	19.3
$\sigma_{PCN}{}^{\dagger}$ [Å]	2.7	2.6	2.5	2.5
$z_{CG}{}^{*}$ [Å]	14.7	15.0	15.6	15.2
$\sigma_{CG}{}^{\dagger}$ [Å]	2.4	2.4	2.5	2.5
$\sigma_{HC}{}^{\dagger}$ [Å]	2.4	2.4	2.4	2.4
$\sigma_{CH3}{}^{\dagger}$ [Å]	2.8	2.9	2.8	2.6
d [Å]	65.19	63.31	65.71	63.46
d_W [Å]	26.2	24.9	26.3	24.9
η	0.08	0.06	0.06	0.1
χ^2	0.65	1.23	0.87	1.31

[*]z_i representing the position of molecular fragments.
[†]σ_i representing the width of Gaussians of molecular fragments.

Table S2: Structural parameters of four different phospholipid bilayers containing $20\,\mathrm{mol}\%$ cholesterol analyzed by SDP-GAP. Parameter uncertainties are estimated to be $< 2\%$ as described in Materials and Methods.

Par	DPPC	POPC	SOPC	DOPC
Temp	$50\,℃$	$30\,℃$	$30\,℃$	$30\,℃$
V_L [$\mathring{A}^3$]	1229	1256	1309	1303
V_{HL} [$\mathring{A}^3$]	331	331	331	331
A [$\mathring{A}^2$]	61.2	63.6	60.7	66.2
d_B [$\mathring{A}$]	40.1	39.5	40.5	39.4
d_{HH} [$\mathring{A}$]	42.3	40.3	42.1	40.9
d_C [$\mathring{A}$]	14.2	14.4	14.9	13.5
$z_{CholCH3}$ [$\mathring{A}$]	22.4	21.7	22.3	21.8
$\sigma_{CholCH3}$ [$\mathring{A}$]	2.98	2.98	2.98	2.98
z_{PCN} [$\mathring{A}$]	21.5	20.7	21.3	20.8
σ_{PCN} [$\mathring{A}$]	2.6	2.6	2.5	2.6
z_{CG} [$\mathring{A}$]	15.1	15.2	15.6	14.1
σ_{CG} [$\mathring{A}$]	2.6	2.6	2.6	2.6
σ_{HC} [$\mathring{A}$]	2.4	2.4	2.4	2.4
σ_{CH3} [$\mathring{A}$]	2.4	2.5	2.6	2.1
d [$\mathring{A}$]	67.48	65.78	67.95	67.46
d_W [$\mathring{A}$]	27.3	26.3	27.4	28.1
η	0.02	0.05	0.05	0.14
χ^2	1.9	0.75	0.99	1.59

Table S3: Structural parameters for POPC at 30 °C using diverse combinations of SAXS and SANS data. Parameter uncertainties are estimated to be < 2% as described in Materials and Methods.

Par	n-ULV$_u$*	n-ULV$_d$†	n-MLV$_u$‡	n-MLV$_d$§	all data¶
A [Å^2]	65.0	63.1	63.6	63.1	63.6
d_B [Å]	38.6	39.8	39.5	39.8	39.5
d_{HH} [Å]	36.8	37.4	37.1	37.3	37.5
d_C [Å]	14.1	14.4	14.6	14.4	14.3
$z_{CholCH3}$ [Å]	20.4	20.9	20.5	20.7	20.9
$\sigma_{CholCH3}$ [Å]	2.98	2.98	2.98	2.98	2.98
z_{PCN} [Å]	19.4	19.9	19.5	19.7	19.9
σ_{PCN} [Å]	2.5	2.6	2.6	2.5	2.6
z_{CG} [Å]	15.0	15.4	15.3	15.4	15.3
σ_{CG} [Å]	2.4	2.4	2.4	2.4	2.4
σ_{HC} [Å]	2.4	2.4	2.4	2.4	2.4
σ_{CH3} [Å]	2.8	2.8	2.8	2.7	2.8

*SAXS (POPC-MLV) and SANS (POPC-ULV) data.
†SAXS (POPC-MLV) and SANS (POPC-d31-ULV) data.
‡SAXS (POPC-MLV) and SANS (POPC-MLV) data.
§SAXS (POPC-MLV) and SANS (POPC-d31-MLV) data.
¶SAXS (POPC-MLVs) and SANS (POPC-ULVs/MLVs, POPC-d31-ULVs/MLVs) data.