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Supporting Material

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The sensitivity of the SDP model to various contrast scattering data

Tests to the SDP model have been performed using simulated form factors, *F(q)*, with *q* values comparable to those from typical experiments, and where appropriate levels of noise were added. X-ray data were subdivided into four *q* ranges ($q<0.3$Å^{-1}; 0.3Å$^{-1}<q<0.5$Å^{-1}; 0.5Å$^{-1}<q<0.6$Å^{-1}; 0.6Å$^{-1}<q<0.8$Å^{-1}), with the added noise increasing with increasing *q*. Neutron data were subdivided into two intervals ($q<0.17$Å^{-1}; 0.17Å$^{-1}<q<0.3$Å^{-1}). The uncertainties assigned to X-ray and neutron *F(q)* were adjusted such that the total weight of all neutron data versus X-ray data corresponded to the ratio of their maximum *q* values (i.e., 0.3:0.8).Test results of SDP model robustness reproduced from Kučerka et al., [Biophys. J. 95, 2356 (2008)] are shown in Table S1.

Table S1: Structural parameters of a diC18:1PC bilayer from MD simulation, and the evaluation of different contrast form factors (calculated) using the SDP model.

	MD simulation	All contrasts	X-ray +Neutron: H_2O/D_2O contrasts	All Neutron contrasts	Neutron: H_2O/D_2O contrasts	X-ray
V_L	1295	1295**	1295**	1295**	1295**	1295**
V_{HL}	319	319**	319**	319**	319**	319**
R_{CG}	0.48	0.45*	0.45*	0.47*	0.47*	0.46*
R_{PCN}	0.27	0.26*	0.26*	0.27*	0.27*	0.28*
r	1.93	1.92*	1.92*	1.94*	1.94*	1.97*
r_{12}	0.81	0.84*	0.83*	0.81*	0.80*	0.76*
D_B	35.8	35.9	35.9	35.9	36.1	35.9
D_{HH}	36.4	35.9	36.0	35.1	33.9	36.1
$2D_C$	27.0	27.0	27.1	27.1	27.2	27.0
D_{H1}	4.7	4.4	4.4	4.0	3.3	4.5
A	72.4	72.2	72.1	72.1	71.8	72.2
Additional Constraints	--	σ_{CH}	σ_{CH}, $\sigma_{CholCH3}$	σ_{CH}, z_{CH}, σ_{CH3}	σ_{CH}, z_{CH}, $\sigma_{CholCH3}$, σ_{CH3}	σ_{CH}, z_{CH}, $\sigma_{CholCH3}$, $z_{CholCH3}$, D_{H1}

diC18:1PC bilayer structural parameters were obtained from a molecular dynamics (MD) simulation [Kučerka et al., Biophys. J. **95,** 2356 (2008)]. From the MD data form factors were calculated for the various contrast data (i.e., X-ray and different neutron contrasts), which were then analyzed using the SDP model. H_2O/D_2O contrasts include nondeuterated lipids in 50% and 100% D_2O. "All neutron contrasts" also includes deuterated lipids (i.e., diC18:1PC_d9, diC18:1PC_d13 and diC18:1PC_d62). Double asterisks denote fixed parameters and single asterisks denote "soft" constrained parameters. Additional soft constrained parameters are also listed in the table. Units for all parameters are Å to the appropriate power.

Table S1 makes it clear that by having fewer data sets, more constraints are needed to fit the data. For example, removing the neutron data of bilayers with selectively deuterated lipids requires an additional constraint be placed to the CholCH3 group - because the remaining data is not optimized to "see" the CholCH3 group. In the case of no X-ray data, it is difficult to clearly distinguish the terminal methyl groups. Surprisingly, in the absence of X-ray data the position of the methine CH groups is also not well determined, and z_{CH} has to be constrained. Finally, when only X-ray data is used, the fit to the data requires the largest number of constraints (X-ray column) - due to the methine CH groups and the choline methyls having poor X-ray contrast. However, bilayer structural parameters are best determined, and with the least number of constraints, when an appropriately parsed model is used in conjunction with neutron and X-ray data.

Application of the SDP model to experimental data

SDP analysis was applied to X-ray and different contrast neutron data, including nondeuterated lipids in 50%, 70% and 100% D_2O. Table S2 presents the list of structural parameters that were determined using the SDP model.

Table S2: Structural parameters of 30°C diCn:1PC bilayers obtained using the SDP model.

Lipid	diC14:1PC	diC16:1PC	diC18:1PC	diC20:1PC	diC22:1PC	diC24:1PC
V_L	1081.2**	1192**	1303**	1413.6**	1524.4**	1635.2**
V_{HL}	331**	331**	331**	331**	331**	331**
R_{CG} (0.48)	0.42*	0.41*	0.39*	0.47*	0.41*	0.43*
R_{PCN} (0.31)	0.27*	0.28*	0.26*	0.26*	0.28*	0.28*
r (1.95)	2.10*	2.07*	2.10*	2.05*	2.00*	1.91*
r_{12} (0.82)	0.80*	0.72*	0.74*	0.84*	0.85*	0.99*
D_B	33.7	36.2	38.9	42.5	46.4	52.2
D_{HH}	29.6	32.1	36.8	38.9	45.5	47.9
$2D_C$	23.4	26.2	29.1	32.5	36.3	41.6
D_{H1}	3.1	3.0	3.9	3.2	4.6	3.1
A	64.2	65.8	66.9	66.6	65.7	62.7
z_{CG}	11.9	13.3	14.5	16.9	18.3	21.1
σ_{CG}	2.40	2.38	2.15	2.68	2.15	2.22
z_{PCN}	15.7	17.1	19.3	20.2	23.1	25.4
σ_{PCN}	2.51	2.59	2.50	3.12	2.14	2.84
$z_{CholCH3}$	17.1	18.3	21.2	21.6	24.2	27.0
$\sigma_{CholCH3}$	2.98**	2.98**	2.98**	2.98**	2.98**	2.98**
z_{CH}	5.70**	7.40**	9.00**	9.00**	9.00**	9.00**
σ_{CH}	3.05**	3.05**	3.05**	3.05**	3.05**	3.05**
σ_{HC} (2.44)	3.02*	2.91*	2.85*	2.93*	2.78*	3.18**
σ_{CH3}	2.54	3.25	3.58	3.84	4.15	3.11

Double asterisks denote fixed parameters and single asterisks denote "soft" constrained parameters. Units for all parameters are Å to the appropriate power.

It is worth noting that D_{HI} in electron density profiles is defined as the distance between the hydrocarbon chain / headgroup interface and the headgroup peak. The latter is usually associated with the position of the electron-dense phosphate group. However, the headgroup peak is comprised of a number of groups (i.e., phosphate, choline, carbonyl and glycerol) that are sitting on top of electron density distributions corresponding to water and hydrocarbon chains. As a result, the positions of the headgroup and phosphate peaks may not necessarily overlap. Our analysis suggests that there may be ~1 Å offset between the phosphate peak represented by the PCN [i.e., the phosphate and part of the choline (CH_2CH_2N)] group and the overall headgroup maximum ($D_{HH}/2$).