

Phospholipid Vesicle Formation in Protic Ionic Liquids

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Supplementary Information

Figures S1-S8 show the scattering patterns and models of best fit for all of the lipid/solvent combinations and temperatures. The parameters for these models of best fit are shown in Tables S1 and S2.

The SFF Model (see ref. 48) does not have a polydispersity component which is why some of the model curves for ULVs display wave-like oscillation that is not present in the scattering data.

Table S2 demonstrates that for the multilamellar vesicles (see ref 47), the repeat spacing (D^*) obtained from fitting was a reasonable match to D^* calculated by the peak position, in most cases.

Figure S9 and Table S3 demonstrate why some of the ranges of possible thickness values are so broad. The parameters of each of the fits are vastly different, as shown in Table S3, and yet the quality of fits are comparable, as shown in Figure S9. For consistency, the parameters reported in Table S1 and S2 are for the parameters that give the best possible fit.

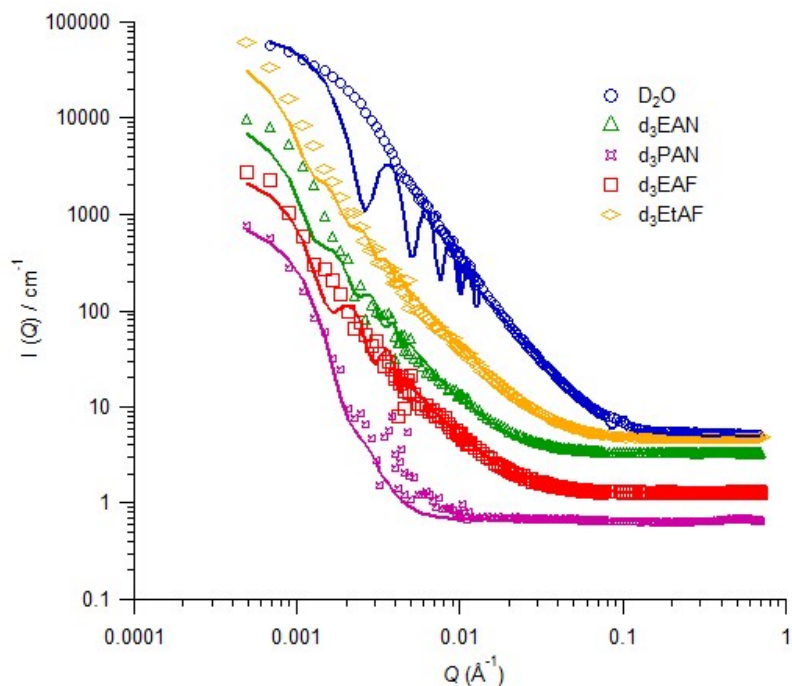


Figure S1. SANS patterns and fitting curves for 0.6 wt% EggPC in D₂O and partially deuterated ionic liquids at 25 °C following the ethanol injection method. Arbitrary offset in the y-axis for clarity. Fitting parameters in Tables S1 & S2.

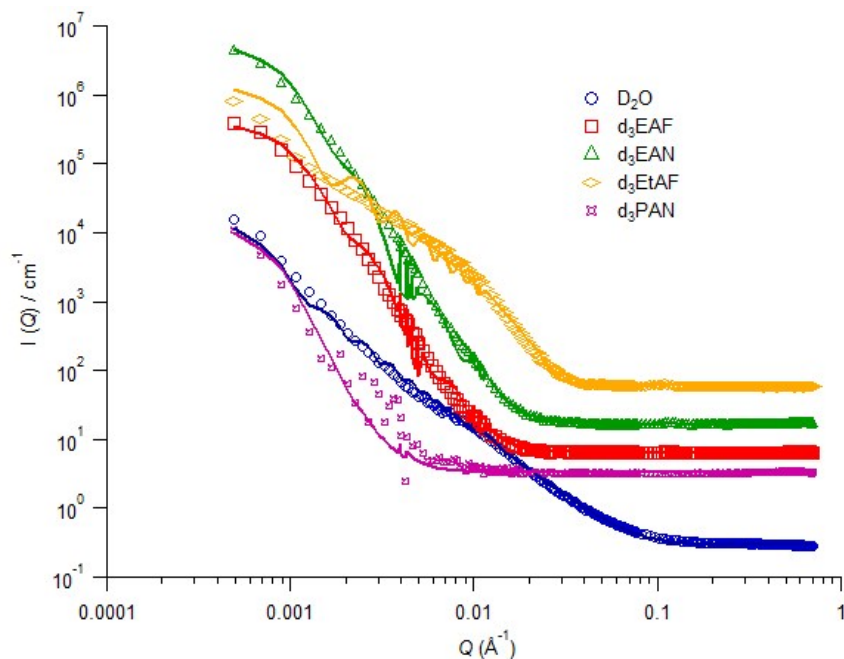


Figure S2. SANS patterns and fitting curves for 0.6 wt% DMPC in D₂O and partially deuterated ionic liquids at 25 °C following the ethanol injection method. Arbitrary offset in the y-axis for clarity. Fitting parameters in Tables S1 & S2.

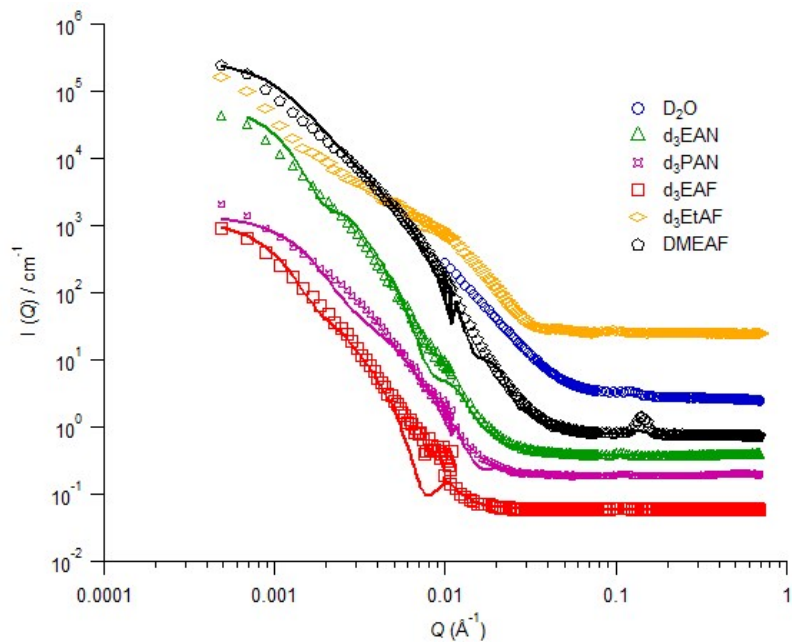


Figure S3. SANS patterns and fitting curves for 0.6 wt% DPPC in D_2O and partially deuterated ionic liquids at 25 °C following the ethanol injection method. Arbitrary offset in the y-axis for clarity. Fitting parameters in Tables S1 & S2.

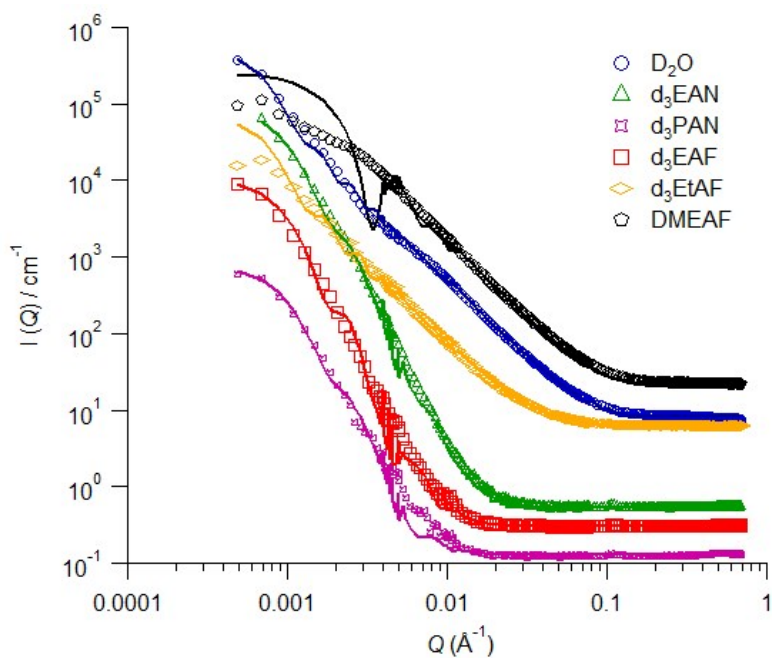


Figure S4. SANS patterns and fitting curves for 0.6 wt% DPPC in D_2O and partially deuterated ionic liquids at 48 °C following the ethanol injection method. Arbitrary offset in the y-axis for clarity. Fitting parameters in Tables S1 & S2.

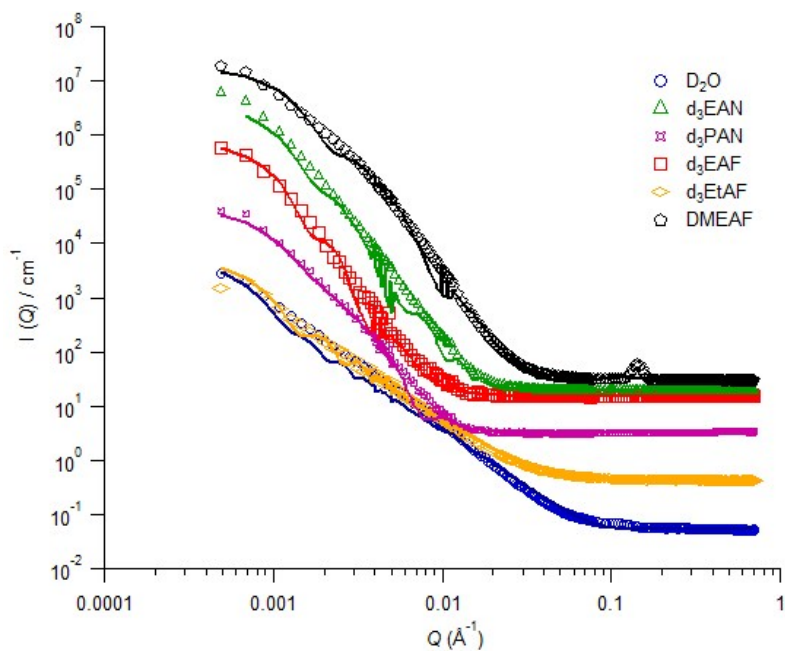


Figure S5. SANS patterns and fitting curves for 0.6 wt% DPPC in D₂O and partially deuterated ionic liquids at 25 °C following the ethanol injection method, and heating to 48 °C. Arbitrary offset in the y-axis for clarity. Fitting parameters in Tables S1 & S2.

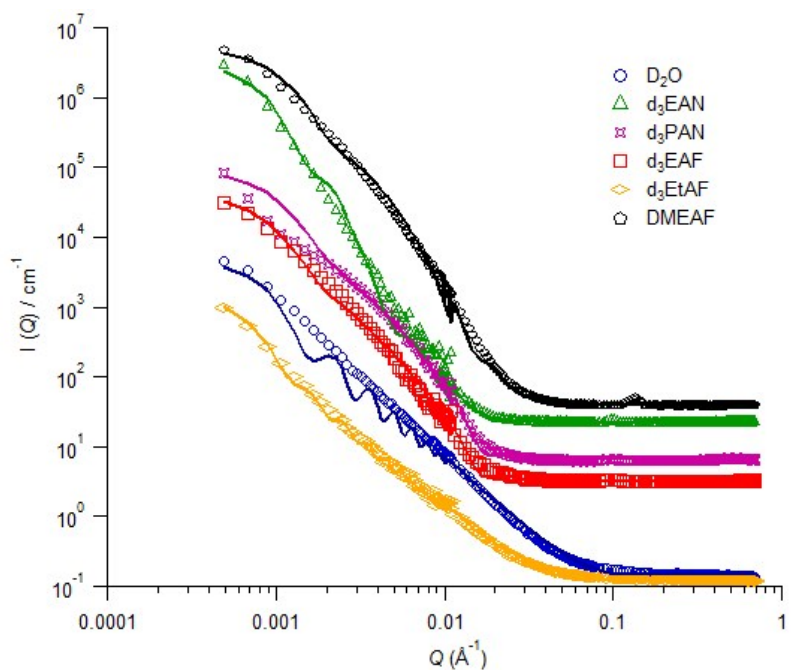


Figure S6. SANS patterns and fitting curves for 0.6 wt% DSPC in D₂O and partially deuterated ionic liquids at 25 °C following the ethanol injection method. Arbitrary offset in the y-axis for clarity. Fitting parameters in Tables S1 & S2.

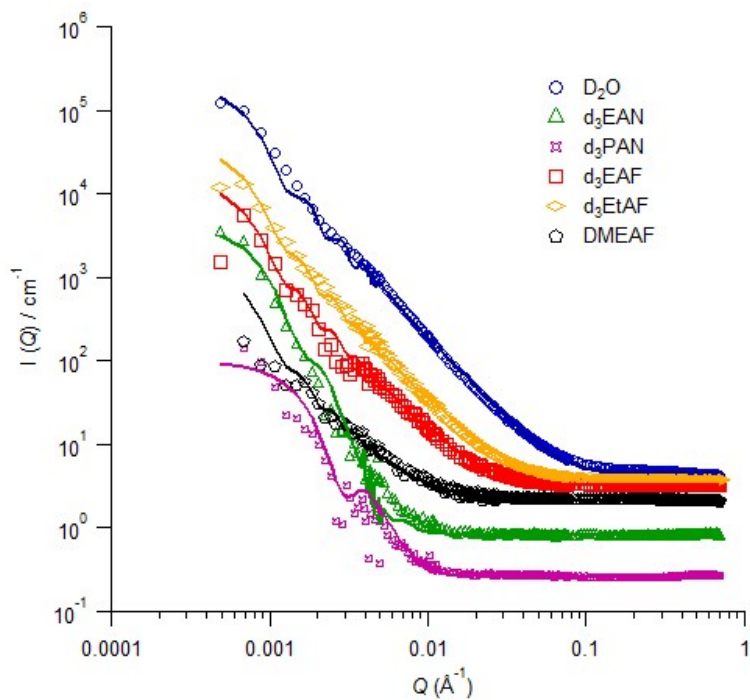


Figure S7. SANS patterns and fitting curves for 0.6 wt% DSPC in D₂O and partially deuterated ionic liquids at 65 °C following the ethanol injection method. Arbitrary offset in the y-axis for clarity. Fitting parameters in Tables S1 & S2.

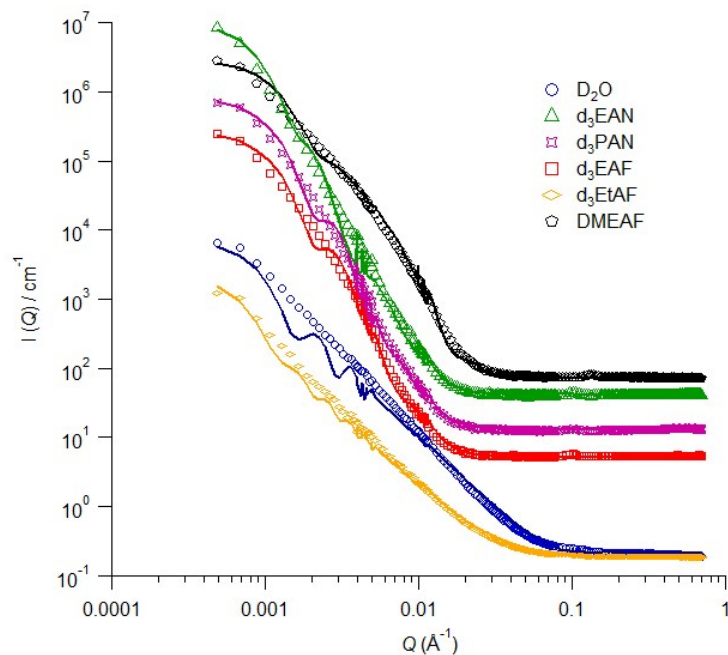


Figure S8. SANS patterns and fitting curves for 0.6 wt% DSPC in D₂O and partially deuterated ionic liquids at 25 °C following the ethanol injection method and heating to 65 °C. Arbitrary offset in the y-axis for clarity. Fitting parameters in Tables S1 & S2.

Table S1. Parameters for separated form factor (SFF) model of best fit for each solvent/lipid combination that had unilamellar vesicles (ULVs). Head group SLD set to 1E-06 (\AA^{-2}) in all cases.

		Bkg (cm^{-1})	Tail width (\AA)	Head width (\AA)	Radius (\AA)	Scale	SLD Tail (\AA^{-2})	SLD Solvent (\AA^{-2})	Total Thickness (\AA)
EggPC	D2O	0.25	25	10	400	0.0200	-2.86E-07	6.30E-06	45.00
EggPC	D2O	0.25	15	5	400	0.0650	-2.86E-07	6.30E-06	25.00
EggPC	EAN	0.64	40	10	900	0.0010	-2.86E-07	3.30E-06	60.00
EggPC	EAF	0.64	35	10	950	0.0018	-2.86E-07	2.55E-06	55.00
EggPC	EtAF	0.58	35	8	1000	0.0034	-2.86E-07	3.14E-06	51.00
DMPC	D2O	0.30	25	10	1000	0.0035	-2.86E-07	6.30E-06	45.00
DPPC 25 °C	D2O	Scattering at 20m not collected							
DPPC 48 °C	D2O	0.27	20	12	1000	0.0050	-2.86E-07	6.30E-06	44.00
DPPC 25 °C rpt	D2O	0.27	40	10	1000	0.0021	-2.86E-07	6.30E-06	60.00
DPPC 25 °C	EtAF	Does not fit well to any models							
DPPC 48 °C	EtAF	0.63	40	10	900	0.0043	-2.86E-07	3.14E-06	60.00
DPPC 25 °C rpt	EtAF	0.62	35	10	800	0.0070	-2.86E-07	3.14E-06	55.00
DPPC 48 °C	DMEAF	0.73	30	10	300	0.2200	6.01E-06	2.90E-07	50.00
DSPC 25 °C	D2O	0.29	37	10	700	0.0036	-2.86E-07	6.30E-06	57.00
DSPC 65 °C	D2O	0.31	31	7	900	0.0032	-2.86E-07	6.30E-06	45.00
DSPC 25 °C rpt	D2O	0.31	40	10	700	0.0035	-2.86E-07	6.30E-06	60.00
DSPC 65 °C	EAF	0.65	50	10	1000	0.0012	-2.86E-07	2.55E-06	70.00
DSPC 25 °C	EtAF	0.60	30	10	1000	0.0048	-2.86E-07	3.14E-06	50.00
DSPC 65 °C	EtAF	0.63	35.0000	15	1000	0.0055	-2.86E-07	3.14E-06	65.00
DSPC 25 °C rpt	EtAF	0.63	30.0000	10	1000	0.0085	-2.86E-07	3.14E-06	50.00
DSPC 65 °C	DMEAF	0.70	20.0000	10	1000	0.0004	6.01E-06	2.90E-07	40.00

Table S2. Parameters for multishell model of best fit for each solvent/lipid combination that had multilamellar vesicles (MLVs). Shell SLD was $-2.86\text{E-}7$ (\AA^{-2}), except in DMEAF when it was $6.01\text{E-}6$ (\AA^{-2}).

		Bkg (cm^{-1})	Scale	Radius (\AA)	Core SLD (\AA^{-2})	No. Pairs	Shell Width	Head Width	Polydisp ersity	D* From Fit (\AA)	D* From Peak (\AA)
DMPC	EAN	0.55	0.0047	992	3.30E-06	30	39.9	15.049	0.40413	54	52
DMPC	EAF	0.64	0.0030	900	2.55E-06	25	35	15	0.39967	50	54
DMPC	EtAF	0.60	0.0100	2000	3.14E-06	10	15	2	0	17	57
DPPC 25 °C	EAN	0.52	0.0046	856	3.30E-06	23	29.824	2.0883	0.4	31	56
DPPC 48 °C	EAN	0.52	0.0030	1000	3.30E-06	23	40.00	10.00	0.48	50	56
DPPC 25 °C rpt	EAN	0.52	0.0030	997	3.30E-06	26	40.01	9.99	0.48	49	56
DPPC 25 °C	PAN	0.64	0.0017	700	2.70E-06	15	23.00	5.00	0.48	28	56
DPPC 48 °C	PAN	0.64	0.0002	1000	2.70E-06	40	23.00	5.00	0.48	28	56
DPPC 25 °C rpt	PAN	0.65	0.0006	894	2.70E-06	31	21.91	5.81	0.67	27	56
DPPC 25 °C	EAF	0.59	0.0010	899	2.50E-06	20	34.19	7.36	0.70	41	No peak
DPPC 48 °C	EAF	0.60	0.0008	1100	2.50E-06	30	40.00	8.63	0.20	48	56
DPPC 25 °C rpt	EAF	0.60	0.0008	1099	2.50E-06	36	40.35	8.71	0.20	49	No peak
DPPC 25 °C	DMEAF	0.75	0.0199	576	2.90E-07	12	34.11	10.14	0.76	44	43
DPPC 25 °C rpt	DMEAF	0.74	0.0170	1000	2.90E-07	14	35.27	12.00	0.30	47	43
DSPC 25 °C	EAN	0.55	0.0017	1500	3.30E-06	20	55.00	10.00	0.20	65	64
DSPC 65 °C	EAN	0.53	0.0010	1500	3.30E-06	25	35.00	15.00	0.20	50	61.96
DSPC 25 °C rpt	EAN	0.54	0.0030	1200	3.30E-06	25	48.70	17.00	0.31	65	61.96
DSPC 25 °C	PAN	0.65	0.0030	1000	2.70E-06	8	40.00	6.03	0.50	46	59.22
DSPC 65 °C	PAN	0.65	0.0001	800	2.70E-06	13	30.00	6.03	0.20	36	No Peak
DSPC 25 °C rpt	PAN	0.65	0.0024	900	2.70E-06	20	49.98	6.01	0.20	56	61
DSPC 25 °C	EAF	0.64	0.0020	1243	2.55E-06	7	56.12	6.25	0.47	62	65
DSPC 25 °C rpt	EAF	0.65	0.0025	1000	2.55E-06	16	50.00	10.00	0.20	60	61
DSPC 25 °C	DMEAF	0.78	0.0060	1014	2.90E-07	12	31.61	8.00	0.38	39	46
DSPC 25 °C rpt	DMEAF	0.72	0.0025	1014	2.90E-07	10	31.61	8.00	0.38	39	46

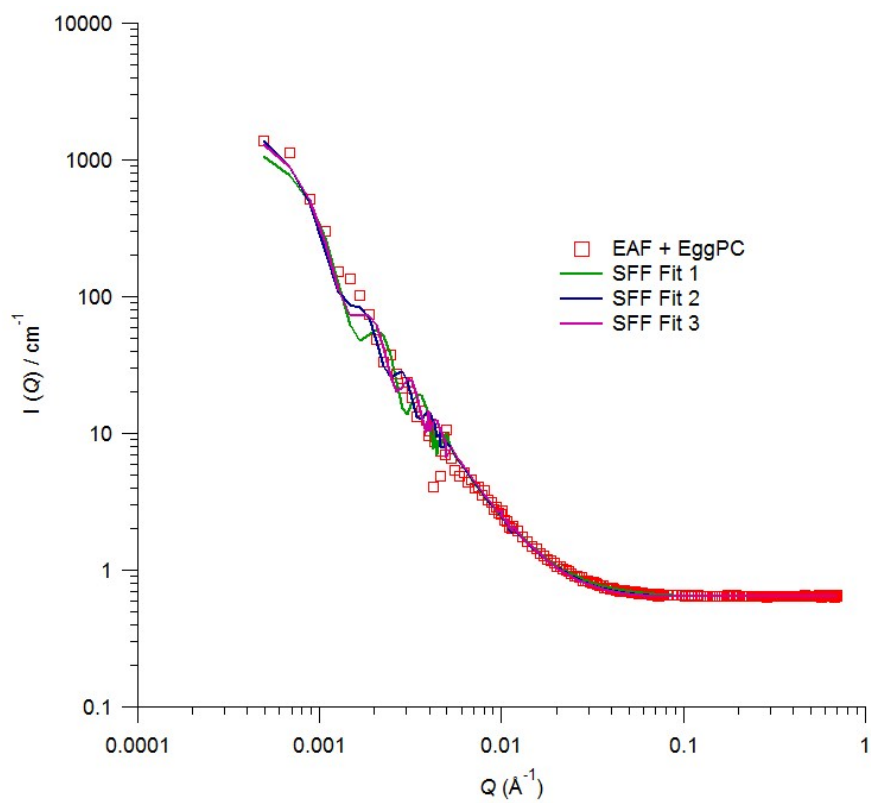


Figure S9. SANS data for EggPC in EAF at 25 °C with three different fits using the SFF model. Parameters for each fit shown in Table S3.

Table S3. Comparison of parameters for three different SFF fits for EggPC in EAF, as modelled in Figure 9.

	Bkg (cm ⁻¹)	Tail width (Å)	Head width (Å)	Radius (Å)	Scale	SLD Tail (Å ⁻²)	SLD Solvent (Å ⁻²)	Total Thickness (Å)
Fit 1	0.64	35	10	950	0.0018	-2.86E-07	2.55E-06	55.00
Fit 2	0.64	55	10	875	0.0010	-2.86E-07	2.55E-06	75.00
Fit 3	0.64	60	15	790	0.0010	-2.86E-07	2.55E-06	90.00