Supporting information to the paper

Small Angle Neutron Scattering Studies of Phospholipid - NSAID Adducts

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Optimization Method and Constraints:

In order to perform fitting of the SFF model to the SANS data, multiobjective optimization program based on Genetic Algorithm called Non-dominated Sorting Genetic Algorithm (NSGA-II) was used[1,2] which was downloaded from Dr. Kalyanmoy Deb's website (http://www.iitk.ac.in/kangal/). The objective to be optimized was the reduced χ^2 defined as,

$$red\,\chi^2 = \frac{1}{N_{data} - f}\sum_{i=1}^{N_{data}}\left[\frac{I_{model} - I_{expt}}{\sigma_{expt}}\right]^2$$

where N_{data} and f are the number of data points and the number of free parameters respectively, along with following constraints,

$$0 < p < 0.6$$
$$d_C, d_H, N_w \text{ and } bkg \text{ are} > 0$$
$$0 < A_L < 70\,\text{Å}^2$$
$$\text{Bilayer Thickness}\left(d_H + d_C\right) \le R_{av}\left(1 - 2p\right)$$
$$300 < R_{av} < 800$$
$$0 < x_{drug} < 1$$

The data at low-q region (q < 0.02 Å^{-1}) is only sensitive to the exact values of vesicle radius and polydispersity while the data in the intermediate-q region (0.02 Å^{-1}< q < 0.2 Å^{-1}) is only sensitive to the bilayer structure.[3] Thus the data was fitted in two regions separately and the physically meaningful values for vesicle radius R_{av} and the polydispersity p were extracted from low-q while that of d_H and N_w were obtained from the intermediate-q region. The low-q data was fitted first for R_{av} and p, which were fixed at these values while doing the fitting at intermediate-q.

Scattering length density profiles from the SFF fitting:

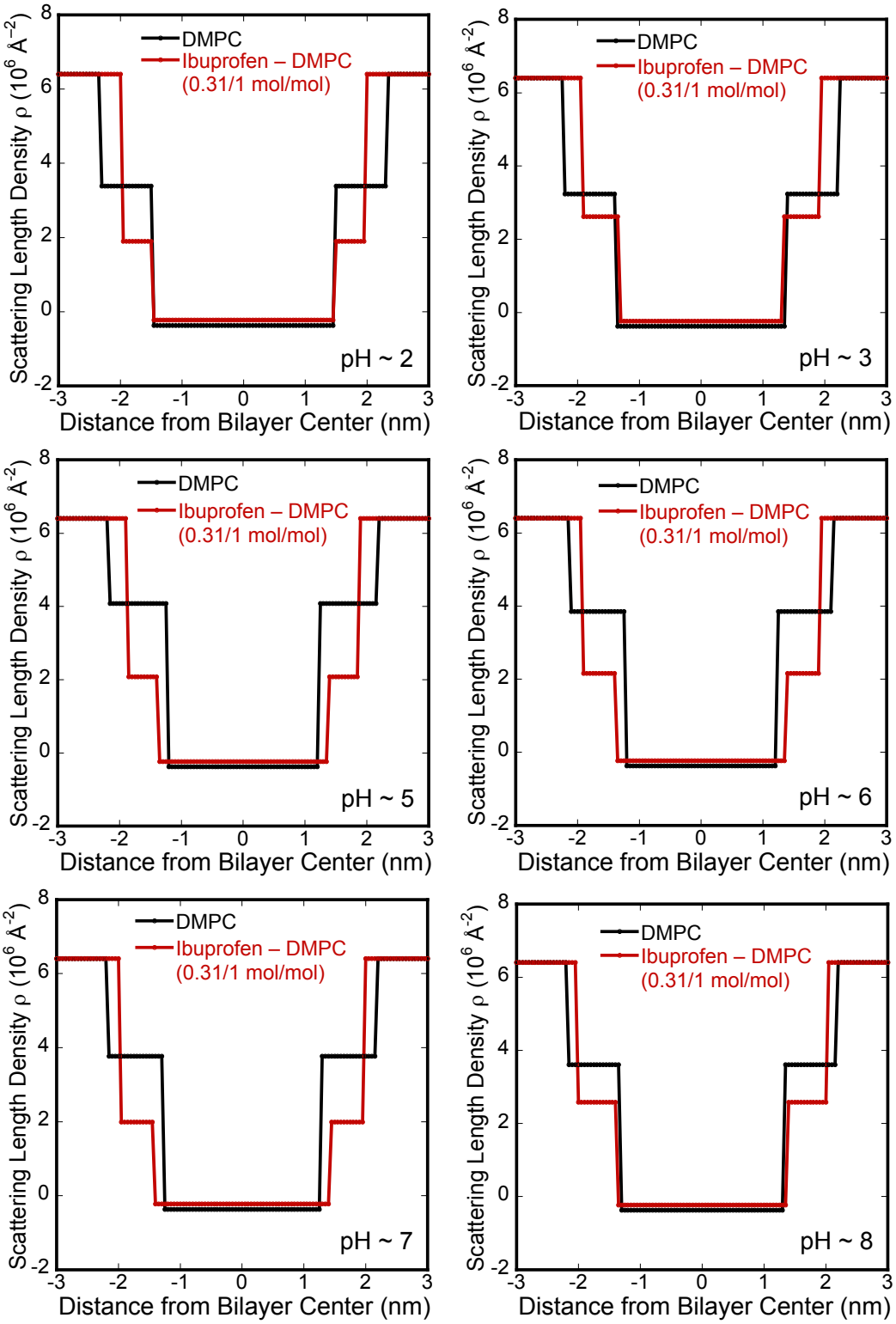

Figure S1. The scattering length density profiles for DMPC and Ibuprofen – DMPC (0.31/1 mol/mol) system at each pH value studied.

Modified Kratky-Porod plots for all pH values:

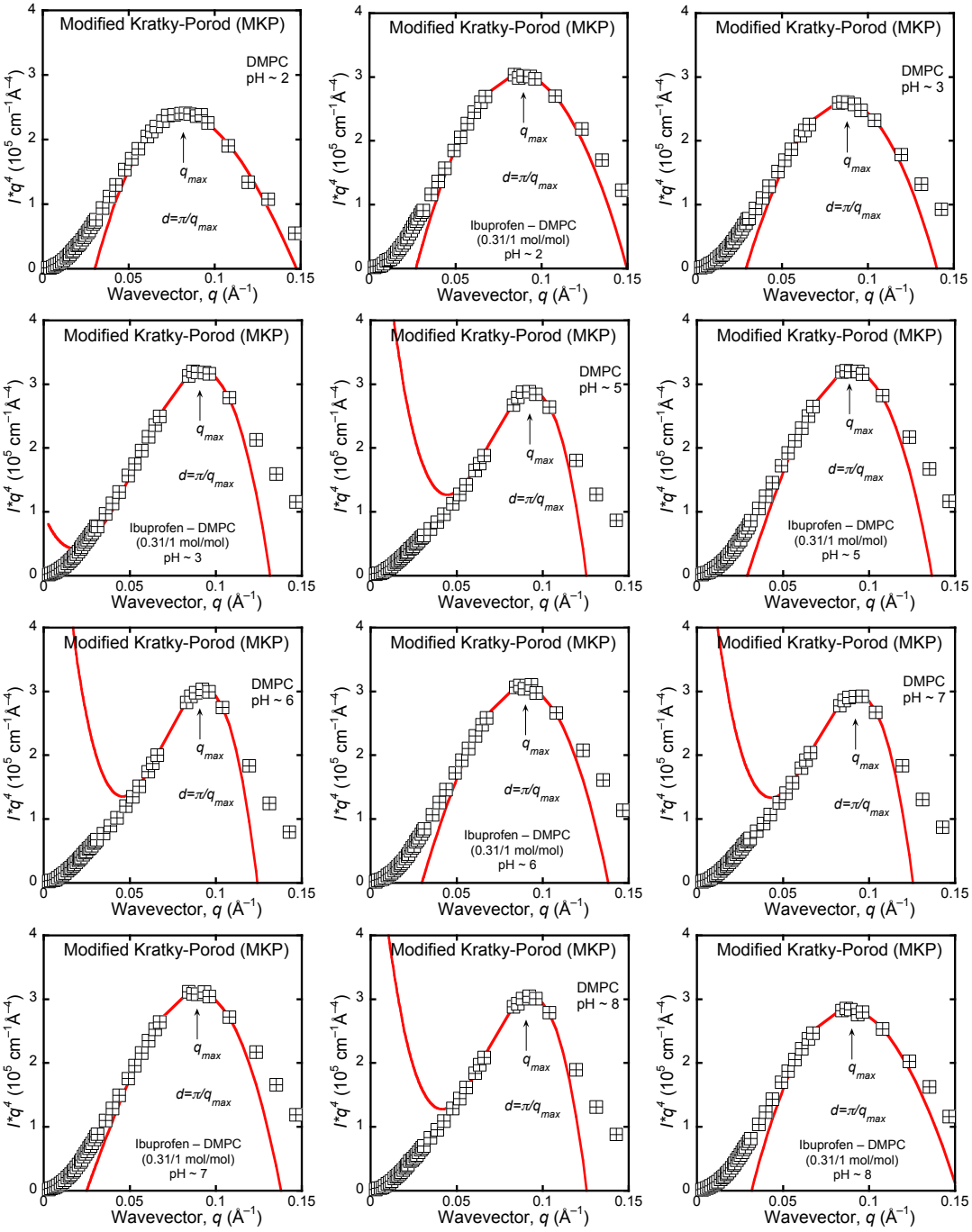

Figure S2. The modified Kratky-Porod (MKP) plots for the DMPC and ibuprofen – DMPC (0.31/1 mol/mol) samples at pH values of ~ 2, 3, 5, 6, 7 and 8.

Table S1. Fitted Parameters from the SFF model.

pH	Ibuprofen – DMPC	R (nm)	p	d_C (nm)	d_H (nm)	t (nm)	A_L (nm^2)	N_w	ρ_H	ρ_C
									10^4 nm^{-2}	
2	0	69.0±0.4	0.2	1.4_5±0.0_2	0.8_9±0.0_4	4.6_9±0.1_1	0.53_8±0.00_6	5.4±0.6	3.3_9±0.1_1	-3.7_2
	0(D54)	58.5±0.4	0.3	1.4_7±0.0_4	0.8_7±0.1_2	4.6_8±0.2_0	0.53_2±0.01_5	4.9±2.9	3.2_3±0.4_3	6.8_2
	0.06	56.7±1.5	0.3	1.4_9±0.0_1	0.6_9±0.0_3	4.3_7±0.0_7	0.53_6±0.00_3	1.8±0.4	2.5_2±0.1_3	-3.4_1
	0.19	55.0±0.4	0.2	1.4_7±0.0_1	0.5_9±0.0_2	4.1_2±0.0_7	0.56_4±0.00_5	0.4±0.4	2.0_6±0.1_4	-2.8_2
	0.31	51.6±0.4	0.2	1.4_5±0.0_1	0.5_4±0.0_1	3.9_8±0.0_4	0.59_4±0.00_6	0.0±0.1	1.9_0±0.0_4	-2.2_8
	0.33(D54)	58.3±8.4	0.2	1.5_0±0.0_2	0.5_5±0.0_1	4.1_2±0.0_6	0.57_7±0.00_8	0.0±0.1	1.8_9±0.0_5	6.2_6
	0.62	52.0±0.3	0.2	1.4_4±0.0_2	0.4_9±0.0_1	3.8_6±0.0_6	0.65_3±0.00_9	0.0±0.2	1.9_1±0.0_8	-1.0_8
3	0	61.5±0.3	0.2	1.4_0±0.0_2	0.8_1±0.0_3	4.4_2±0.0_9	0.56_0±0.00_7	4.6±0.4	3.2_3±0.0_8	-3.7_2
	0.31	58.1±2.9	0.3	1.3_2±0.0_2	0.5_8±0.0_4	3.8_1±0.1_2	0.65_4±0.01_1	2.1±0.7	2.6_2±0.1_9	-2.2_8
5	0	53.4±0.6	0.2	1.2_1±0.0_2	0.9_6±0.0_4	4.3_4±0.1_2	0.64_7±0.01_1	10.1±0.5	4.0_8±0.0_6	-3.7_2
	0.31	54.7±1.3	0.3	1.3_7±0.0_2	0.5_3±0.0_3	3.7_9±0.0_9	0.63_1±0.00_7	0.5±0.5	2.0_8±0.1_7	-2.2_8
6	0	53.0±1.1	0.3	1.2_5±0.0_2	0.9_0±0.0_3	4.3_0±0.0_9	0.62_8±0.00_8	8.3±0.5	3.8_5±0.0_6	-3.7_2
	0.31	48.9±2.6	0.3	1.4_0±0.0_1	0.5_5±0.0_3	3.8_9±0.0_8	0.61_7±0.00_6	0.7±0.5	2.1_6±0.1_7	-2.2_8
7	0	51.1±0.9	0.3	1.2_7±0.0_2	0.8_9±0.0_4	4.3_3±0.1_1	0.61_4±0.00_8	7.6±0.6	3.7_7±0.0_9	-3.72
	0.31	55.6±3.4	0.3	1.4_2±0.0_2	0.5_4±0.0_2	3.9_1±0.0_6	0.60_8±0.00_6	0.3±0.3	1.9_9±0.1_2	-2.2_8
8	0	51.9±1.0	0.3	1.3_1±0.0_2	0.8_6±0.0_4	4.3_4±0.1_1	0.59_9±0.00_7	6.6±0.6	3.6_1±0.1_0	-3.7_2
	0(D54)	58.2±0.9	0.3	1.4_2±0.0_3	0.9_8±0.0_8	4.8_0±0.1_3	0.55_2±0.01_4	7.5±1.8	3.7_2±0.2_3	6.8_2
	0.06	57.1±2.1	0.3	1.3_8±0.0_1	0.6_8±0.0_2	4.1_3±0.0_7	0.57_7±0.00_4	2.4±0.4	2.7_2±0.1_0	-3.4_1
	0.19	60.0±3.1	0.3	1.4_3±0.0_2	0.6_1±0.0_3	4.0_7±0.0_9	0.58_2±0.00_6	1.2±0.5	2.3_4±0.1_5	-2.8_2
	0.31	54.4±4.8	0.3	1.4_0±0.0_2	0.6_2±0.0_4	4.0_3±0.1_0	0.61_6±0.00_8	2.0±0.6	2.5_8±0.1_7	-2.2_8
	0.33(D54)	47.2±0.3	0.4	1.5_2±0.0_2	0.5_6±0.0_1	4.1_7±0.0_6	0.57_0±0.00_9	0.0±0.2	1.9_0±0.0_8	6.2_6
	0.62	51.7±5.3	0.4	1.4_4±0.0_2	0.4_9±0.0_2	3.8_6±0.0_7	0.65_4±0.01_1	0.0±0.2	1.9_1±0.0_7	-1.0_8

1. Deb, K. *Multi-Objective Optimization Using Evolutionary Algorithms*, 1st ed.; John Wiley & Sons: New York, 2001.
2. Deb, K.; Pratap, A.; Agarwal, S.; Meyarivan, T. *IEEE Transac. Evolut. Comp.* **2002,** *6*, 182-197.
3. Kučerka, N.; Nagle, J. F.; Feller, S. E.; Balgavý, P. M. *Phys. Rev. B* **2004,** *69*, 51903.