Electronic Supplementary Information for

Calcium-mediated binding of DNA to 1,2-distearoyl-sn-glycero-3phosphocholine-containing mixed lipid monolayers

Aleksandra P. Dabkowska, David J. Barlow, Luke A. Clifton, Arwel V. Hughes, John R.P. Webster, Rebecca J. Green, Peter J. Quinn and M. Jayne Lawrence



Supplementary Figure 1. Surface tension of ultrapure water (black square), 20 mM $CaCl_2$ (red circles) and 0.067 mg mL⁻¹ ctDNA in aqueous 20 mM $CaCl_2$ measured over time on a Kruss tensiometer. The points are a mean of 3 measurements with the error bars representing the standard deviation.

Electronic Supplementary Material (ESI) for Soft Matter This journal is © The Royal Society of Chemistry 2014



Supplementary Figure 2. Comparison of the external reflection FTIR spectra of lipid monolayers at 10 mN m⁻¹ (red) and 30 mN m⁻¹ (black) on a sub-phase of 20 mM CaCl₂. The spectral regions of the CH₂ stretch vibrations (2820-2960 cm⁻¹) are shown for (a) DSPC, (c) DSPC/cholesterol, and (e) DSPC/DOPE monolayers. The phosphate stretch vibrations (900 to 1300 cm⁻¹) are shown for (b) DSPC, (d) DSPC/cholesterol, and (f) DSPC/DOPE monolayers.

Electronic Supplementary Material (ESI) for Soft Matter This journal is © The Royal Society of Chemistry 2014



Supplementary Figure 3. Comparison of the external reflection FTIR spectra of lipid monolayers at 10 mN m⁻¹ (red) and 30 mN m⁻¹ (black) on a sub-phase of 20 mM CaCl₂ with calf thymus DNA (0.067 mg mg mL⁻¹). The spectral regions of the CH₂ stretch vibrations (2820-2960 cm⁻¹) are shown for (a) DSPC, (c) DSPC/cholesterol, and (e) DSPC/DOPE monolayers. The phosphate stretch vibrations (900 to 1300 cm⁻¹) are shown for (b) DSPC, (d) DSPC/cholesterol, and (f) DSPC/DOPE monolayers.

Electronic Supplementary Material (ESI) for Soft Matter This journal is © The Royal Society of Chemistry 2014



Supplementary Figure 4. Comparison of the external reflection FTIR spectra of lipid monolayers at 295 ± 2 K and at a surface pressure of 10 mN m⁻¹ on a subphase of 20 mM CaCl₂ without (black line) and with (red line) calf thymus DNA (0.067 mg mL⁻¹). The spectral regions of the CH₂ stretch vibrations (2820-2960 cm⁻¹) are shown for (a) DSPC, (c) DSPC/cholesterol, and (e) DSPC/DOPE monolayers. The phosphate stretch vibrations (900 to 1300 cm⁻¹) are shown for (b) DSPC, (d) DSPC/cholesterol, and (f) DSPC/DOPE monolayers.

Electronic Supplementary Material (ESI) for Soft Matter This journal is C The Royal Society of Chemistry 2014

Supplementary Table 1. Integrated peak areas of the CH_2 asymmetrical and symmetrical stretches and PO_2^- asymmetrical and symmetrical starching modes.

Vibrational Mode				
Sample	CH ₂ assym	CH ₂ sym	PO_2 assym	PO ₂ sym
	(2885-2946 cm ⁻¹)	(2835-2870 cm ⁻¹)	(1275-1190 cm ⁻¹)	(1130-1020 cm ⁻¹)
DSPC 10 mN m ⁻¹	0.0846	0.0342	0.0497	0.1223
DSPC + DNA 10 mN m ⁻¹	0.0744	0.0295	0.0752	0.2138
DSPC 30 mN m ⁻¹	0.0966	0.0353	0.0618	0.1227
DSPC + DNA 30 mN m ⁻¹	0.0948	0.0347	0.0921	0.2243
DSPC/cholesterol 10 mN m ⁻¹	0.0721	0.0262	0.0230	0.0407
DSPC/cholesterol + DNA 10 mN m ⁻¹	0.0831	0.0309	0.0520	0.0955
DSPC/cholesterol 30 mN m ⁻¹	0.0756	0.0299	0.055	0.0517
DSPC/cholesterol + DNA 30 mN m ⁻¹	0.0773	0.0332	0.0817	0.1179
DSPC/DOPE 10 mN m ⁻¹	0.053	0.022	0.0348	0.04
DSPC/DOPE + DNA 10 mN m ⁻¹	0.047	0.02	0.057	0.085
DSPC /DOPE 30 mN m ⁻¹	0.074	0.028	0.036	0.046
DSPC/DOPE + DNA 30 mN m ⁻¹	0.053	0.025	0.074	0.0147



Supplementary Figure 5. SNR profiles for DSPC/cholesterol on a 20 mM CaCl₂ sub-phase at the surface pressures of (A) 10 mN m⁻¹, (B) 20 mN m⁻¹ and (C) 40 mN m⁻¹ fitted using a two layer model. The contrasts shown are chain-deuterated lipid on acmw (•), fully-deuterated lipid on acmw (Δ) and protiated lipid on D₂O (O). The simultaneous, three-layer fit is shown as a solid line (—) on each contrast.



Supplementary Figure 6. SNR profiles for DSPC/DOPE on a 20 mM CaCl₂ sub-phase at the surface pressures of (A) 10 mN m⁻¹ and (B) 20 mN m⁻¹ fitted using a two layer model. The contrasts shown are chain-deuterated lipid on acmw (\bullet), fully-deuterated lipid on acmw (\triangle) and protiated lipid on D₂O (O). The simultaneous, three-layer fit is shown as a solid line (—) on each contrast.



Supplementary Figure 7. SNR profiles for DSPC/cholesterol on a 20 mM CaCl₂ sub-phase containing ctDNA (0.067 mg mL⁻¹) at the surface pressures of (A) 10 mN m⁻¹, (B) 20 mN m⁻¹ and (C) 40 mN m⁻¹ fitted using a two layer model. The contrasts shown are chain-deuterated lipid on acmw (\bullet), fully-deuterated lipid on acmw (Δ) and protiated lipid on D₂O (O). The simultaneous, three-layer fit is shown as a solid line (—) on each contrast.



Supplementary Figure 8. SNR profiles for DSPC/DOPE on a 20 mM CaCl₂ sub-phase containing ctDNA (0.067 mg mL⁻¹) at the surface pressures of (A) 10 mN m⁻¹ and (B) 20 mN m⁻¹ fitted using a two layer model. The contrasts shown are chain-deuterated lipid on acmw (\bullet), fully-deuterated lipid on acmw (Δ) and protiated lipid on D₂O (O). The simultaneous, three-layer fit is shown as a solid line (—) on each contrast.