

Nanoparticle Wettability Influences Nanoparticle–Phospholipid Interactions

Online Supplement

Nagarjun V. Konduru ^{a,b}, Flavia Damiani ^a, Svetla Stoilova-McPhie ^c, Jason S. Tresback ^c,
Georgios Pyrgiotakis ^{a,b} Thomas C. Donaghey ^{a,b}, Philip Demokritou ^{a,b}, Joseph D. Brain ^{a,b},
Ramon M. Molina ^{a,b} §

^a Molecular and Integrative Physiological Sciences Program, Department of Environmental Health, Harvard T.H. Chan School of Public Health, 665 Huntington Avenue, Boston, MA 02115, USA.

^b Center for Nanotechnology and Nanotoxicology, Harvard T.H. Chan School of Public Health, 665 Huntington Avenue, Boston, MA 02115, USA.

^c Center for Nanoscale Systems, Faculty of Art and Sciences, Harvard University, 11 Oxford Street, Cambridge, MA, 02138, USA.

Corresponding Author:

§ Ramon M. Molina, Molecular and Integrative Physiological Sciences Program, Harvard Department of Environmental Health, School of Public Health, 665 Huntington Avenue, Boston, MA 02115, USA. Tel: 617-432-2311

Email: rmolina@hsph.harvard.edu

Table S1. Tandem quadruple mass spectroscopic analysis of phospholipid from rat BAL fluid and of extracted phospholipids from nanoparticle surface after incubation in cell-free rat alveolar lavage fluid at 37°C for 30 minutes.

A. Phosphatidylcholine (Data are ng phospholipid bound per mg nanoparticles. Blank cells indicate not detectable)

Compound	Rat BALf (µg/ml)	CeO₂	Si-CeO₂	BaSO₄	ZnO
C14:0	0.02	2.93	4.21	0.52	5.15
C16:0e				0.68	1.35
C16:1			0.68		
C16:0	0.41	158.19	146.18	72.89	192.12
C18:2					6.16
C18:1					3.89
C18:0		33.68	25.74	17.21	35.36
C20:4		4.63	3.12	1.85	3.95
C22:6		4.97	2.29	2.71	2.79
C30:1e	0.01	2.25	1.66	1.85	2.67
C30:0e	0.1	32.71	31.13		
C30:1	0.70	256.41	186.81	120.09	198.33
C32:3	0.25	13.10	6.22	5.10	12.57
C32:2	3.22	228.18	91.68	136.68	285.63
C32:1	28.84	3163.16	1667.18	1994.94	3823.13
C32:0	82.94	33972.09	23902.62	19225.14	38472.62
C34:3e		5.24	2.35		2.52
C34:1e		11.86	6.53	4.42	6.91
C34:4	0.25	10.69		5.75	11.84
C34:3	1.71	143.32	64.02	84.37	142.53
C34:2	20.91	1404.68	624.24	802.32	1560.20
C34:1	9.95	750.49	362.89	461.80	917.95
C34:0	4.05	629.67	474.02	336.97	761.64
C36:4e		3.82		2.50	5.21
C36:6	0.05				1.36
C36:5	1.44	61.06	27.04	31.92	58.67
C36:4	4.93	363.16	169.57	224.25	441.23
C36:3	1.18	42.37	23.91	30.43	56.53
C36:2	3.87	127.99	70.69	42.90	95.64
C36:1	0.70		19.63	10.87	13.28
C36:0					
C38:6e	5.68	11.26	7.47	8.27	16.35
C38:6	2.52	174.69	73.02	85.76	168.94

C38:5	1.08	43.82	19.02	22.36	40.13
C38:4	1.82	69.06	33.66	34.86	80.32
C38:1		40.86	25.47	19.29	32.54
C40:8	0.20	3.47	2.00	1.86	4.28
C40:7			2.29	1.26	2.26
C40:6	0.49	15.69	10.06	7.90	18.43
C40:5	0.53		3.82		7.78
C40:1		2.52			1.05
Total LPC		204.39	182.22	95.86	250.77
Total PC		41583.64	27909.00	23703.85	47242.55

B. Phosphatidylethanolamine (Data are ng phospholipid bound per mg nanoparticles. Blank cells indicate not detectable)

Compound	Rat BALf ($\mu\text{g/ml}$)	CeO ₂	Si-CeO ₂	BaSO ₄	ZnO
C14:0			0.02	0.01	
C16:1		0.07	0.09	0.04	
C16:0		0.79	0.66	0.62	0.47
C18:2				0.02	0.10
C18:1		0.08	0.06	0.04	0.12
C18:0		0.74	0.43	0.30	0.62
C20:4		0.06	0.03	0.03	0.08
C22:6		0.06	0.05	0.04	0.09
C22:4		0.02	0.01	0.01	0.02
C34:2p / C34:3e		0.95	1.14	0.54	0.82
C34:3		2.02	1.24	1.82	3.79
C34:2		20.82	13.80	17.34	42.17
C34:1		37.17	19.75	24.42	44.01
C34:0			2.63		
C36:4p / C36:5e		2.85	1.72	1.29	4.31
C36:3p / C36:2e		1.76	1.60	1.27	2.81
C36:6		0.31	0.21	0.18	0.36
C36:5	0.40	3.94	2.15	3.17	6.58
C36:4		26.09	15.40	22.71	43.08
C36:3		4.46	1.89	3.24	6.91
C36:2		1.88	1.89	4.62	18.01
C36:1		8.03	3.55	4.13	8.90
C38:5p / C38:6e		3.71	3.10	3.02	4.27
C38:6	4.10	17.18	11.76	11.83	22.65
C38:5		9.93	5.92	8.74	15.55
C38:4	0.45	13.96	8.28	11.36	23.89
C38:3		1.26	0.55	0.40	1.25
C40:8		0.30		0.19	0.28
C40:7		1.60	0.90	1.42	2.22

C40:6		4.46	3.40	3.89	6.37
C40:5		2.02	0.86	1.28	3.15
C40:4		1.67	0.96	1.04	2.43
C40:1		0.09	0.09	0.11	0.16
Total LPE		1.81	1.35	1.12	1.49
Total PE		166.45	102.81	128.00	263.96

C. Phosphatidylinositol (Data are ng phospholipid bound per mg nanoparticles. Blank cells indicate not detectable)

Compound	Rat BALf ($\mu\text{g/ml}$)	CeO ₂	Si-CeO ₂	BaSO ₄	ZnO
C32:2	0.80	2.63		0.92	2.04
C32:1		15.13	6.43	6.06	13.02
C34:2		96.66	54.59	49.90	83.57
C34:1	0.48	39.61	24.14	23.73	34.24
C34:0		25.93	16.75		15.15
C36:5		9.18	3.12	4.11	4.37
C36:4	0.53	48.50	17.77	21.10	34.03
C36:3	0.70	17.90		6.42	13.42
C36:2	1.23	48.37	19.16	24.58	39.93
C36:1				9.52	12.44
C38:6	0.95	148.20	78.73	57.48	90.09
C38:5	0.58	40.46		18.90	26.78
C38:4	1.13	54.30	18.06	29.13	43.98
C40:6	0.71	15.72	12.61	10.69	15.88
C40:5				4.06	
Total LPI					
Total PI		562.58	251.34	266.59	428.93

D. Phosphatidylglycerol (Data are ng phospholipid bound per mg nanoparticles. Blank cells indicate not detectable)

Compound	Rat BALf ($\mu\text{g/ml}$)	CeO ₂	Si-CeO ₂	BaSO ₄	ZnO
C16:1					0.04
C16:0	0.06	1.06	0.77	0.61	1.10
C18:3					0.02
C18:2		0.57	0.24	0.60	0.97
C18:1		0.54	0.30	0.31	0.91
C18:0	0.04	0.48	0.26	0.25	0.61
C22:6					0.02
C34:1	0.38	18.47	17.16	11.79	51.94
C36:5		18.62	19.65	10.35	36.21
C36:4	0.81	87.31	65.14	54.15	159.21

C36:3	0.66	12.56	31.16	10.37	42.86
C36:2	1.46	21.04	23.59	12.34	41.84
C36:1		8.77	4.89	3.31	20.44
C38:6		111.90	148.09	69.43	207.56
C38:5		37.85	51.68	23.97	69.53
C38:4	0.05	14.56	9.83	6.18	26.07
Total LPG		2.65	1.58	1.77	3.67
Total PG		331.08	371.19	201.90	655.65

E. Phosphatidylserine (Data are ng phospholipid bound per mg nanoparticles. Blank cells indicate not detectable)

Compound	Rat BALf (µg/ml)	CeO ₂	Si-CeO ₂	BaSO ₄	ZnO
C18:0		0.09	0.06	0.06	0.08
C34:2		2.74	0.82	1.21	2.56
C34:1	0.65	9.16	5.95	5.85	12.34
C34:0		8.68	7.86	6.28	11.18
C36:4		0.88	0.44	0.63	1.22
C36:3					1.05
C36:2		12.55	7.46	8.37	18.92
C36:1	0.66	52.97	38.49	34.90	73.93
C38:6					0.28
C38:5		0.43		0.73	1.99
C38:4		10.04	6.00	6.75	12.76
C38:3		2.39	1.58	1.50	4.62
C38:2		1.04		0.62	1.75
C38:1		2.23	1.10	1.15	2.41
C40:7					0.31
C40:6		5.37	3.41	3.14	5.91
C40:5		1.86	1.77	1.61	3.22
C40:4		3.18	1.98	2.50	5.28
Total LPS		0.09	0.06	0.06	0.08
Total PS		113.52	76.88	75.22	159.76

F. Phosphatidic acid (Data are ng phospholipid bound per mg nanoparticles. Blank cells indicate not detectable)

Compound	Rat BALf (µg/ml)	CeO ₂	Si-CeO ₂	BaSO ₄	ZnO
18:0 LPA		28.09	16.71	10.76	22.08
C32:0		8.35		2.54	2.15
C36:0		6.78	3.41	1.91	1.08
C38:6		80.72	35.04	37.82	29.57
C38:5	0.26	2007.73	1070.24	845.50	630.26

C38:4	0.05	143.95	93.28	66.29	49.60
C40:6	0.04	211.13	79.26	74.28	59.17
C40:5		116.76	52.14	39.77	30.36
Total LPA		28.09	16.71	10.76	22.08
Total PA		2575.42	1333.37	1068.11	802.20

G. Sphingomyelin (Data are ng phospholipid bound per mg nanoparticles. Blank cells indicate not detectable)

Compound	Rat BALf ($\mu\text{g/ml}$)	CeO₂	Si-CeO₂	BaSO₄	ZnO
C32:0 SM	0.05				
C34:0 SM	0.00				
C36:1 SM	2.46				
C36:0 SM	24.91				
C38:2 SM	1.72				
C38:1 SM	12.02				
C38:0 SM	8.93				
C40:3 SM	3.23				
C42:4 SM	0.49				
C42:3 SM	1.73				

Figure S1. A cryo-TEM image of rat bronchoalveolar lavage fluid showing large sheets of lipid bilayers in micron sizes covering multiple holes of the grid.

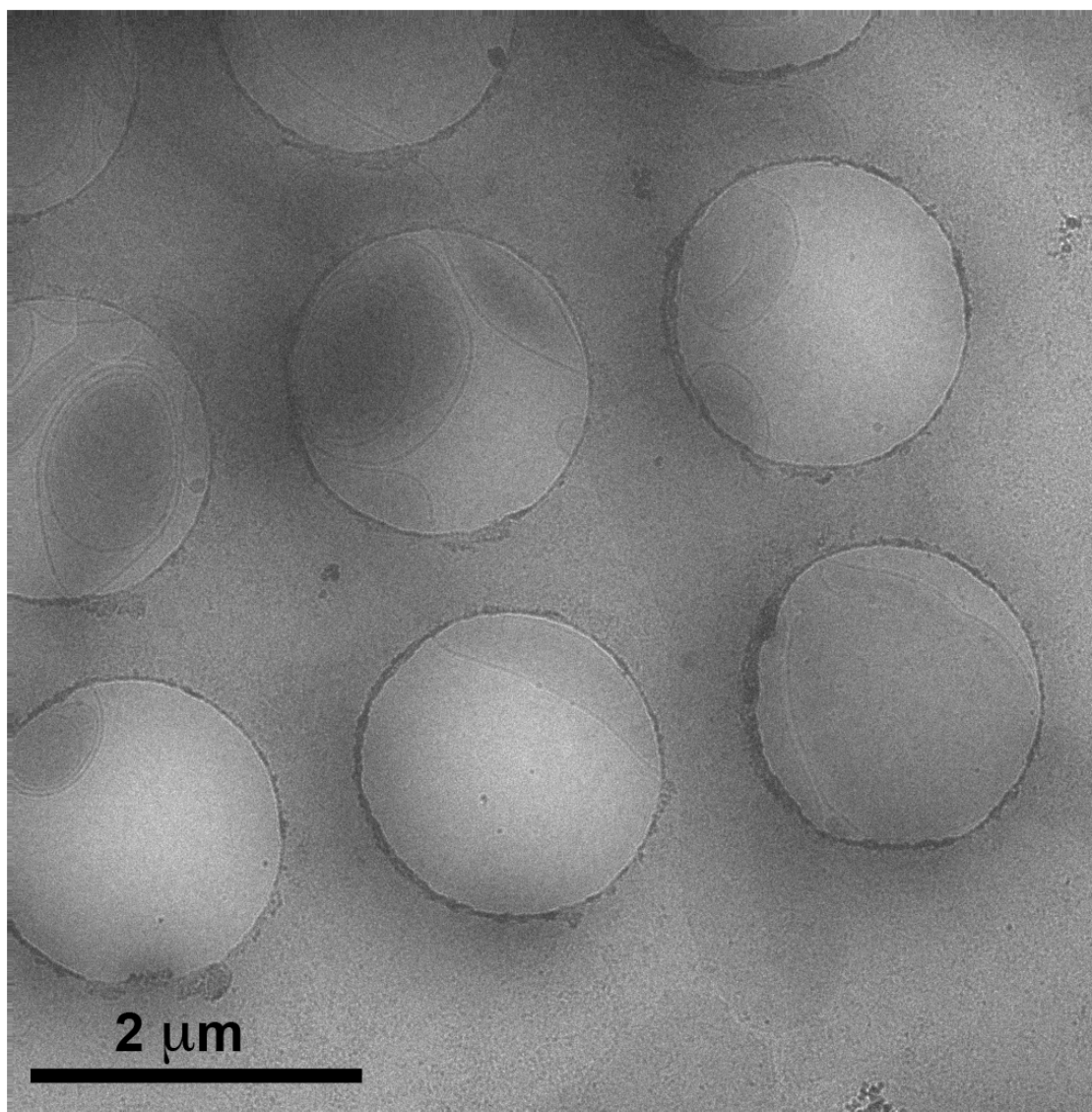


Figure S2. AFM height and phase contrast images of CeO₂ (**a, b**) and BaSO₄ (**c, d**) NPs post-incubation in 2:1 mixture of DPPC and DPPA lipids. Height images: CeO₂ (**a**) and BaSO₄ (**c**). Phase images: CeO₂ (**b**) and BaSO₄ (**d**).

