Electronic Supplementary Material (ESI) for Soft Matter

Biomimetic membrane control of block copolymer vesicles with tunable wall thickness

Supplementary Information

Mengying Xiao,[a] Jiannan Liu,[b] Jiexin Yang,[b] Rong Wang*[b] and Daiqian Xie*[a]

[a] Institute of Theoretical and Computational Chemistry, Key Laboratory of Mesoscopic Chemistry, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210093, China

[b] Department of Polymer Science and Engineering, State Key Laboratory of Coordination Chemistry, Nanjing National Laboratory of Microstructures, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210093, China

Email: rong_wang73@hotmail.com, dqxie@nju.edu.cn

Electronic Supplementary Material (ESI) for Soft Matter

Table S1. Summary of the vesicle (micelle) sizes and cavity sizes with corresponding wall thicknesses for six groups of vesicles with a_{BS} = 75 at t = 12000.

N	r_{cavity}	d_{inner}	d	d_{outer}	R
		$A_1B_5A_1$ block copolymer			
679	1.0	0.3	2.1	0.5	3.9
805	1.1	0.3	2.4	0.3	4.1
1211	1.5	0.4	2.7	0.4	5.0
1309	1.6	0.4	2.9	0.5	5.4
1596	1.8	0.4	3.0	0.4	5.6
2499	1.7	0.4	4.4	0.4	6.9
		$A_1B_7A_1$ block copolymer			
125					2.4
486	0.6	0.3	2.2	0.4	3.5
657	0.7	0.3	2.7	0.4	4.1
810	0.8	0.3	2.8	0.3	4.2
820	0.9	0.3	2.7	0.4	4.3
828	0.6	0.4	3.1	0.4	4.5
828	0.9	0.3	3.2	0.4	4.8
1566	1.5	0.3	3.4	0.4	5.6
1980	1.8	0.3	3.4	0.4	5.9
		$A_1B_9A_1$ block copolymer			

242					2.5
385	0.5	0.1	2.3	0.4	3.2
627	0.6	0.4	2.5	0.5	4.0
1100	0.7	0.3	3.6	0.2	4.8
1716	1.5	0.2	3.6	0.2	5.5
1903	1.2	0.4	3.7	0.3	5.6
2123	1.6	0.3	3.6	0.3	5.8
$A_1B_{11}A_1$ block copolymer					
182					2.5
468	0.4	0.2	2.7	0.3	3.6
676	0.6	0.3	2.6	0.4	3.9
728	0.6	0.3	2.6	0.4	4.0
858	0.8	0.3	2.8	0.4	4.3
923	0.6	0.3	3.2	0.3	4.4
2067	1.6	0.2	3.5	0.4	5.7
2197	1.5	0.3	3.6	0.5	5.9
$A_1B_{13}A_1$ block copolymer					
360					3.3
480	0.2	0.1	2.9	0.4	3.6
1080	0.7	0.5	3.2	0.5	4.9
1365	0.8	0.3	3.9	0.3	5.3
2235	1.3	0.4	4.0	0.5	6.2

2580	1.4	0.3	4.3	0.4	6.5
$A_1B_{15}A_1$ block copolymer					
493					3.6
918	0.6	0.4	3.3	0.5	4.8
1139	0.8	0.4	3.2	0.4	4.8
1394	0.8	0.6	3.3	0.5	5.2
1666	1.1	0.6	3.4	0.5	5.6
2482	1.5	0.3	3.7	0.5	6.0

Table S2. Summary of the vesicle (micelle) sizes and cavity sizes with corresponding wall thicknesses for six groups of vesicles with a_{BS} = 110 at t = 12000.

N	r_{cavity}	d_{inner}	d	d_{outer}	R
		$A_1B_5A_1$ block copolymer			
196	0.4	0.2	1.7	0.3	2.6
707	0.8	0.5	2.4	0.5	4.2
721	1.0	0.3	2.4	0.4	4.1
742	1.0	0.4	2.4	0.5	4.3
812	1.2	0.4	2.1	0.5	4.2
791	1.1	0.3	2.3	0.5	4.2
1085	1.4	0.3	2.4	0.5	4.6
3045	2.4	0.4	3.7	0.6	7.1
		$A_1B_7A_1$ block copolymer			
297	0.4	0.2	2.3	0.3	3.2
333	0.3	0.3	2.2	0.2	3.0
387	0.3	0.3	2.3	0.4	3.3
441	0.5	0.3	2.3	0.4	3.5
522	0.8	0.2	2.2	0.4	3.6
621	0.8	0.3	2.4	0.5	4.0
747	0.9	0.4	2.5	0.4	4.2
1287	1.4	0.2	3.1	0.5	5.2

1476	1.5	0.2	3.2	0.5	5.4
1989	1.1	0.4	3.9	0.4	5.9
		$A_1B_9A_1$ block copolymer			
781	1.0	0.2	2.6	0.4	4.2
836	0.7	0.4	2.6	0.4	4.1
836	0.9	0.3	2.6	0.4	4.2
946	0.7	0.4	3.1	0.3	4.5
1034	0.8	0.4	3.2	0.2	4.6
3663	2.1	0.3	4.2	0.4	7.0
		$A_1B_{11}A_1$ block copolymer			
195	0.5				2.7
572	0.4	0.4	2.6	0.4	3.8
884	0.7	0.3	3.0	0.3	4.3
1144	0.9	0.5	3.0	0.4	4.8
1495	1.0	0.3	3.4	0.3	5.0
1716	1.2	0.3	3.6	0.4	5.5
2093	1.6	0.3	3.7	0.2	5.8
		$A_1B_{13}A_1$ block copolymer			
375					3.1
630	0.4	0.1	3.3	0.2	4.0
765	0.6	0.3	3.0	0.3	4.2
900	0.6	0.4	2.9	0.4	4.3

1320	0.9	0.3	3.3	0.5	5.0
1995	1.2	0.3	3.8	0.4	5.7
2115	1.4	0.4	3.7	0.3	5.8
$A_1B_{15}A_1$ block copolymer					
357	0.3				3.1
765	0.6	0.1	3.1	0.2	4.0
1411	0.6	0.5	3.5	0.3	4.9
1513	1.2	0.2	3.5	0.3	5.2
1921	1.1	0.3	4.1	0.3	5.8
2125	0.9	0.4	4.2	0.3	5.8

Table S3. The variation of the area densities of the A-block in both coronas with the vesicle size with $a_{BS} = 75$ at $t = 12000$.

N	r_{cavity} (r_i)	N_i	$N_i/4\pi r_i^2$	R (r_o)	N_o	$N_o/4\pi r_o^2$
			$A_1B_5A_1$ block copolymer			
679	1.0	53	4.2176	3.9	141	0.7377
805	1.1	62	4.0775	4.1	168	0.7953
1211	1.5	109	3.8550	5.0	237	0.7543
1309	1.6	124	3.8545	5.4	250	0.6822
1596	1.8	157	3.8560	5.6	299	0.7587
2499	1.7	263	7.2418	6.9	451	0.7538
			$A_1B_7A_1$ block copolymer			
125				2.4		
486	0.6	17	3.7578	3.5	91	0.5911
657	0.7	34	5.5217	4.1	112	0.5302
810	0.8	40	4.9735	4.2	140	0.6315
820	0.9	43	4.2244	4.3	139	0.5982
828	0.6	36	7.9577	4.5	148	0.5816
828	0.9	43	4.2244	4.8	141	0.4870
1566	1.5	106	3.7489	5.6	242	0.6140
1980	1.8	141	3.4630	5.9	299	0.6835
			$A_1B_9A_1$ block copolymer			

242				2.5		
385	0.5	5	1.5915	3.2	65	0.5051
627	0.6	13	2.8736	4.0	101	0.5023
1100	0.7	46	7.4705	4.8	154	0.5319
1716	1.5	84	2.9708	5.5	228	0.5997
1903	1.2	96	5.3051	5.6	250	0.6343
2123	1.6	112	3.4815	5.8	274	0.6481
$A_1B_{11}A_1$ block copolymer						
182				2.5		
468	0.4	4	1.9894	3.6	68	0.41754
676	0.6	10	2.2104	3.9	94	0.4918
728	0.6	12	2.6525	4.0	100	0.4973
858	0.8	20	2.4868	4.3	112	0.4820
923	0.6	23	5.0841	4.4	119	0.4891
2067	1.6	82	2.5489	5.7	236	0.5780
2197	1.5	88	3.1123	5.9	250	0.5715
$A_1B_{13}A_1$ block copolymer						
360				3.3		
480	0.2	1	1.9894	3.6	63	0.3868
1080	0.7	24	3.8976	4.9	120	0.3977
1365	0.8	30	3.7301	5.3	152	0.4306
2235	1.3	65	3.0606	6.2	233	0.4823

2580	1.4	79	3.2074	6.5	265	0.4991
$A_1B_{15}A_1$ block copolymer						
493				3.6		
918	0.6	9	1.9894	4.8	99	0.3419
1139	0.8	14	1.7407	4.8	120	0.4144
1394	0.8	23	2.8598	5.2	141	0.4149
1666	1.1	33	2.1702	5.6	163	0.4136
2482	1.5	57	2.0159	6.0	235	0.5194

Table S4. The variation of the area densities of the A-block in both coronas with the vesicle size with $a_{BS} = 110$ at $t = 12000$.

N	r_{cavity} (r_i)	N_i	$N_i/4\pi r_i^2$	R (r_o)	N_o	$N_o/4\pi r_o^2$
			$A_1B_5A_1$ block copolymer			
196	0.4	4	1.9894	2.6	52	0.6121
707	0.8	52	6.4656	4.2	150	0.6766
721	1.0	55	4.3767	4.1	151	0.7148
742	1.0	59	4.6950	4.3	153	0.6584
812	1.2	65	3.5920	4.2	167	0.7533
791	1.1	59	3.8802	4.2	167	0.7533
1085	1.4	98	3.9788	4.6	212	0.7972
3045	2.4	328	4.5314	7.1	542	0.8556
			$A_1B_7A_1$ block copolymer			
297	0.4	3	1.4920	3.2	63	0.4895
333	0.3	6	5.3051	3.0	68	0.6012
387	0.3	9	7.9577	3.3	77	0.5626
441	0.5	13	4.1380	3.5	85	0.5521
522	0.8	22	2.7354	3.6	94	0.5771
621	0.8	27	3.3571	4.0	111	0.5520
747	0.9	39	3.8315	4.2	127	0.5729
1287	1.4	78	3.1668	5.2	208	0.6121

1476	1.5	100	3.5367	5.4	228	0.6222
1989	1.1	132	8.6811	5.9	310	0.7086
$A_1B_9A_1$ block copolymer						
781	1.0	28	2.2281	4.2	114	0.5142
836	0.7	31	5.0344	4.1	121	0.5728
836	0.9	28	2.7508	4.2	124	0.5593
946	0.7	33	5.3593	4.5	139	0.5462
1034	0.8	37	4.6005	4.6	151	0.5678
3663	2.1	219	3.9518	7.0	448	0.7275
$A_1B_{11}A_1$ block copolymer						
195	0.5			2.7		
572	0.4	6	2.9841	3.8	82	0.4518
884	0.7	18	2.9232	4.3	118	0.5078
1144	0.9	21	2.0631	4.8	155	0.5353
1495	1.0	41	3.2626	5.0	189	0.6016
1716	1.2	55	3.0394	5.5	209	0.5498
2093	1.6	80	2.4868	5.8	242	0.5724
$A_1B_{13}A_1$ block copolymer						
375				3.1		
630	0.4	3	1.4920	4.0	81	0.4028
765	0.6	12	2.6525	4.2	90	0.4060
900	0.6	12	2.6525	4.3	108	0.4648

1320	0.9	18	1.7683	5.0	158	0.5029
1995	1.2	51	2.8183	5.7	215	0.5266
2115	1.4	61	2.4766	5.8	221	0.5227
			$A_1B_{15}A_1$ block copolymer			
357	0.3			3.1		
765	0.6	1	0.2210	4.0	89	0.4426
1411	0.6	16	3.5367	4.9	150	0.4971
1513	1.2	26	1.4368	5.2	152	0.4473
1921	1.1	21	1.3811	5.8	205	0.4849
2125	0.9	31	3.0455	5.8	219	0.5180

Table S5. The bridge fraction Φ_b of the obtained vesicles at t = 12000.

a_{BS} = 75				a_{BS} = 110			
N	**bridge**	**loop**	Φ_b	***N***	**bridge**	**loop**	Φ_b
$A_1B_5A_1$ block copolymer							
679	53	44	0.5463	196	4	24	0.1428
805	62	53	0.5391	707	52	49	0.5148
1211	109	64	0.6300	721	55	48	0.5339
1309	124	63	0.6631	742	59	47	0.5566
1596	157	71	0.6886	812	65	51	0.5603
2499	263	94	0.7366	791	59	54	0.5221
				1085	98	57	0.6322
				3045	328	107	0.7540
$A_1B_7A_1$ block copolymer							
125				297	3	30	0.0909
486	17	37	0.3148	333	6	31	0.1621
657	34	39	0.4657	387	9	34	0.2093
810	40	50	0.4444	441	13	36	0.2653
820	43	48	0.4725	522	22	36	0.3793
828	36	56	0.3913	621	27	42	0.3913
828	43	49	0.4673	747	39	44	0.4698
1566	106	68	0.6092	1287	78	65	0.5454

1980	141	79	0.6409	1476	100	64	0.6097
				1989	132	89	0.5972
$A_1B_9A_1$ block copolymer							
242				781	28	43	0.3943
385	5	30	0.1428	836	31	45	0.4078
627	13	44	0.2280	836	28	48	0.3684
1100	46	54	0.4600	946	33	53	0.3837
1716	84	72	0.5384	1034	37	57	0.3936
1903	96	77	0.5549	3663	219	114.5	0.6566
2123	112	81	0.5803				
$A_1B_{11}A_1$ block copolymer							
182				195			
468	4	32	0.1111	572	6	38	0.1363
676	10	42	0.1923	884	18	50	0.2647
728	12	44	0.2142	1144	21	67	0.2386
858	20	46	0.3030	1495	41	74	0.3565
923	23	48	0.3239	1716	55	77	0.4166
2067	82	77	0.5157	2093	80	81	0.4968
2197	88	81	0.5207				
$A_1B_{13}A_1$ block copolymer							
360				375			
480	1	31	0.0312	630	3	39	0.0714

1080	24	48	0.3333	765	12	39	0.2352
1365	30	61	0.3296	900	12	48	0.2000
2235	65	84	0.4362	1320	18	70	0.2045
2580	79	93	0.4593	1995	51	82	0.3834
				2115	61	80	0.4326
$A_1B_{15}A_1$ block copolymer							
493				357			
918	9	45	0.1666	765	1	44	0.0222
1139	14	53	0.2089	1411	16	67	0.1927
1394	23	59	0.2804	1513	26	63	0.2921
1666	33	65	0.3367	1921	21	92	0.1858
2482	57	89	0.3904	2125	31	94	0.2480