SUPPORTING INFORMATION

Molecular Simulations and Understanding of Antifouling Zwitterionic Polymer Brushes

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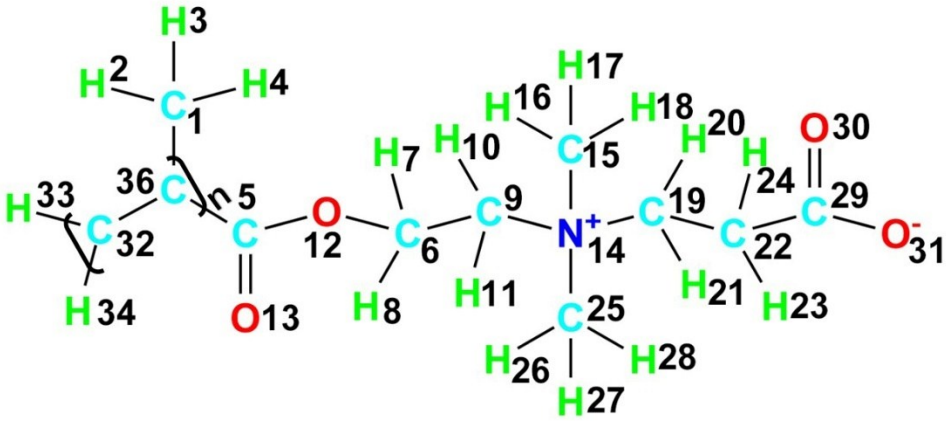
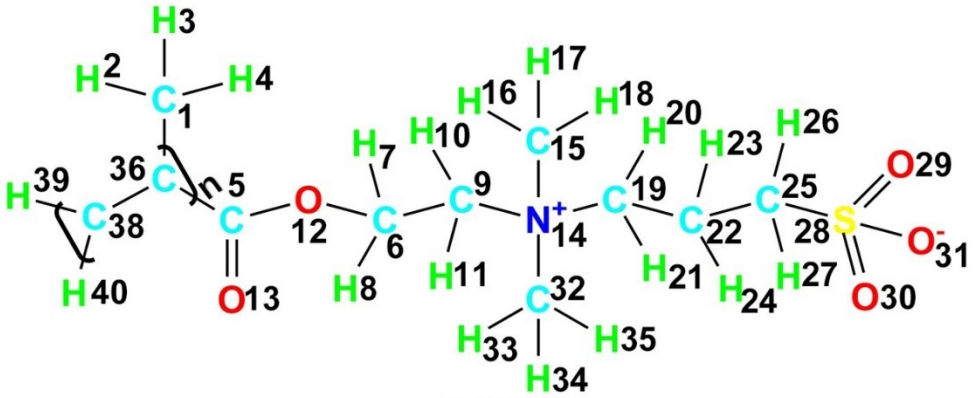
Table S1. Force field parameters of pCBMA, pSBMA, and pMPC in the CHARMM format.



pCBMA

Atom Name	Atom Type	Partial Charge	Epsilon	Rmin/2
C1	CH31	-0.272	-0.078	2.050
H2	HGA3	0.090	-0.024	1.340
H3	HGA3	0.090	-0.024	1.340
H4	HGA3	0.090	-0.024	1.340
C5	CGO2	0.929	-0.098	1.700
C6	CH21	0.080	-0.560	2.010
H7	HGA2	0.090	0.035	1.340
H8	HGA2	0.090	-0.035	1.340
C9	CH24	-0.10	-0.055	2.175
H10	HGP5	0.250	-0.046	0.700
H11	HGP5	0.250	-0.046	0.700
O12	OG02	-0.488	-0.100	1.650
O13	O2D1	-0.638	-0.120	1.700
N14	N3P0	-0.604	-0.200	1.850
C15	CH34	-0.349	-0.077	2.215
H16	HGP5	0.250	-0.046	0.700
H17	HGP5	0.250	-0.046	0.700
H18	HGP5	0.250	-0.046	0.700
C19	CH24	-0.094	-0.055	2.175
H20	HGP5	0.250	-0.046	0.700
H21	HGP5	0.250	-0.046	0.700
C22	CH21	-0.252	-0.560	2.010
H23	HGA2	0.090	0.035	1.340
H24	HGA2	0.090	-0.035	1.340
C25	CH34	-0.349	-0.077	2.215
H26	HGP5	0.250	-0.046	0.700
H27	HGP5	0.250	-0.046	0.700
H28	HGP5	0.250	-0.046	0.700
C29	CGO3	0.587	-0.060	2.000

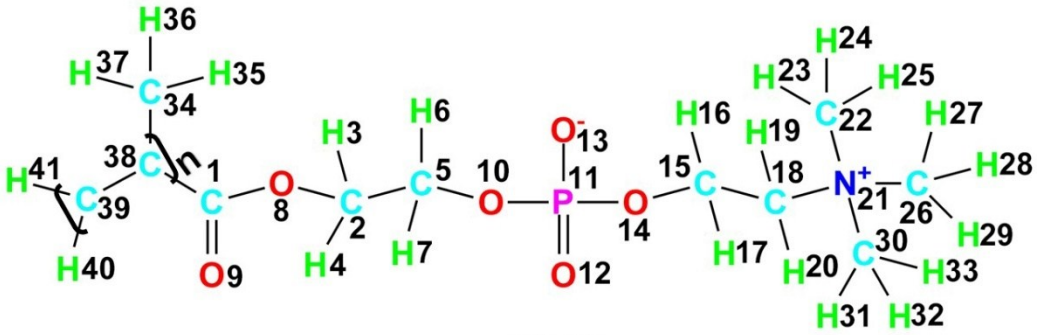
O30	O2D2	-0.760	-0.120	1.700
O31	O2D2	-0.760	-0.120	1.700
C32	CH21	-0.182	-0.560	2.010
H33	HGA2	0.090	0.035	1.340
H34	HGA2	0.090	-0.035	1.340
C36	CH01	-0.058	-0.032	2.000



pSBMA

Atom Name	Atom Type	Partial Charge	Epsilon	Rmin/2
C1	CH31	-0.272	-0.078	2.050
H2	HGA3	0.09	-0.024	1.340
H3	HGA3	0.09	-0.024	1.340
H4	HGA3	0.09	-0.024	1.340
C5	CGO2	0.929	-0.098	1.700
C6	CH21	0.08	-0.560	2.010
H7	HGA2	0.090	0.035	1.340
H8	HGA2	0.090	-0.035	1.340
C9	CH24	-0.100	-0.055	2.175
H10	HGP5	0.250	-0.046	0.700
H11	HGP5	0.250	-0.046	0.700
O12	OG02	-0.488	-0.100	1.650
O13	O2D1	-0.638	-0.120	1.700
N14	N3P0	-0.597	-0.200	1.850
C15	CH34	-0.349	-0.077	2.215
H16	HGP5	0.250	-0.046	0.700
H17	HGP5	0.250	-0.046	0.700
H18	HGP5	0.250	-0.046	0.700
C19	CH24	-0.106	-0.055	2.175
H20	HGP5	0.250	-0.046	0.700
H21	HGP5	0.250	-0.046	0.700
C22	CH21	-0.179	-0.560	2.010
H23	HGA2	0.090	0.035	1.340
H24	HGA2	0.090	-0.035	1.340
C25	CH21	-0.261	-0.560	2.010

H26	HGA2	0.090	0.035	1.340
H27	HGA2	0.090	-0.035	1.340
S28	S3O1	0.730	-0.470	2.100
O29	O2P1	-0.550	-0.120	1.700
O30	O2P1	-0.550	-0.120	1.700
O31	O2P1	-0.550	-0.120	1.700
C32	CH34	-0.349	-0.077	2.215
H33	HGP5	0.250	-0.046	0.700
H34	HGP5	0.250	-0.046	0.700
H35	HGP5	0.250	-0.046	0.700
C36	CH01	-0.058	-0.032	2.000
C38	CH21	-0.182	-0.560	2.010
H39	HGA2	0.090	0.035	1.340
H40	HGA2	0.090	-0.035	1.340



pMPC

Atom Name	Atom Type	Partial Charge	Epsilon	Rmin/2
C1	CGO2	0.929	-0.098	1.700
C2	CH21	0.08	-0.560	2.010
H3	HGA2	0.09	0.035	1.340
H4	HGA2	0.09	-0.035	1.340
C5	CH21	-0.078	-0.560	2.010
H6	HGA2	0.09	0.035	1.340
H7	HGA2	0.09	-0.035	1.340
O8	OG02	-0.489	-0.100	1.650
O9	O2D1	-0.638	-0.120	1.700
O10	OG03	-0.57	-0.100	1.650
P11	PG11	1.498	-0.585	2.150
O12	O2P1	-0.781	-0.120	1.700
O13	O2P1	-0.781	-0.120	1.700
O14	OG03	-0.57	-0.100	1.650
C15	CH21	-0.078	-0.560	2.010
H16	HGA2	0.09	0.035	1.340
H17	HGA2	0.09	-0.035	1.340
C18	CH24	-0.099	-0.055	2.175

H19	HGP5	0.25	-0.046	0.700
H20	HGP5	0.25	-0.046	0.700
N21	N3P0	-0.604	-0.200	1.850
C22	CH34	-0.349	-0.077	2.215
H23	HGP5	0.25	-0.046	0.700
H24	HGP5	0.25	-0.046	0.700
H25	HGP5	0.25	-0.046	0.700
C26	CH34	-0.349	-0.077	2.215
H27	HGP5	0.25	-0.046	0.700
H28	HGP5	0.25	-0.046	0.700
H29	HGP5	0.25	-0.046	0.700
C30	CH34	-0.349	-0.077	2.215
H31	HGP5	0.25	-0.046	0.700
H32	HGP5	0.25	-0.046	0.700
H33	HGP5	0.25	-0.046	0.700
C34	CH21	-0.182	-0.560	2.010
H35	HGA2	0.09	0.035	1.340
H36	HGA2	0.09	-0.035	1.340
C38	CH01	-0.058	-0.032	2.000
C39	CH31	-0.272	-0.078	2.050
H40	HGA3	0.09	-0.024	1.340
H41	HGA3	0.09	-0.024	1.340
H42	HGA3	0.09	-0.024	1.340