

Supporting Information

Decoupling the functional roles of cationic and hydrophobic groups in the antimicrobial and hemolytic activities of methacrylate random copolymers

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1. ¹H NMR spectrum of AE34HE29E37 and assignments
2. Polymer characterization, MIC (*E. coli*) and hemolysis

1. ^1H NMR spectrum of AE34HE29E37 and assignments

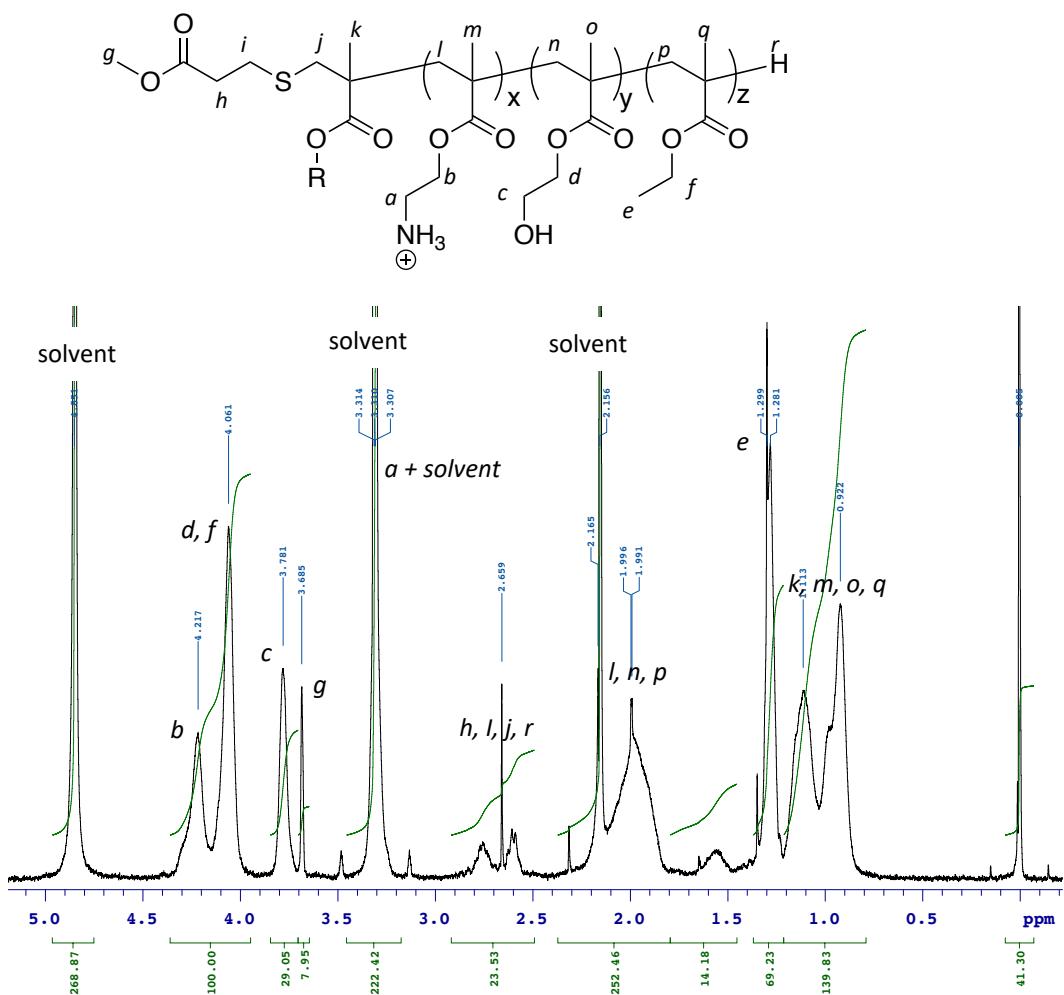


Fig. S1. ^1H NMR of AE34HE29E37.

The DP and mol. % of monomers were determined by the following calculations:

$$\text{DP} = 100/2 (b, d, f) / 7.95/3 (g) = 19$$

$$\text{HEMA} = 29.05 \text{ (c) / 100 (b, d, f)} = 29 \text{ mol.\%}$$

AEMA = $b / (b + d + f) = 27.5 \text{ mm} / (27.5\text{mm} + 53 \text{ mm})^* = 34 \text{ mol.\%}$ (* the heights of integration curve)

$$\text{EMA} = 100 \text{ mol.\%} - 29 \text{ mol.\% (HEMA)} - 34 \text{ mol.\% (AEMA)} = 37 \text{ mol.\%}$$

2. Polymer characterization, MIC (*E. coli*) and hemolysis

Table S1. Characterization of de-protected copolymers with EMA 0 mol. %

Polymer	HEMA ^a (mol. %)	AEMA ^a (mol. %)	EMA ^a (mol. %)	DP	M_n (NMR) w/TFA	M_n (NMR) w/o TFA	MIC <i>E.coli</i> ($\mu\text{g/mL}$)
1	22 (20)	78 (80)	0 (0)	14	3200	2000	>1000
2	38 (40)	62 (60)	0 (0)	16	3300	2200	>1000
3	59 (60)	41 (40)	0 (0)	19	3400	2600	>1000
4	75 (80)	25 (20)	0 (0)	10	1700	1400	>1000
5	100 (100)	0 (0)	0 (0)	23	3100	3100	>1000

a) The values of mol. % of TMS-HEMA, Boc-AEMA, EMA (feed compositions) are given in parentheses.

Table S2. Characterization of de-protected copolymers with EMA 10 mol. %

Polymer	HEMA ^a (mol. %)	AEMA ^a (mol. %)	EMA ^a (mol. %)	DP	M_n (NMR) w/TFA	M_n (NMR) w/o TFA	MIC <i>E. coli</i> ($\mu\text{g/mL}$)
6	0 (0)	87.7 (90)	12.3 (10)	14.9	3510	2030	>1000
7	16 (15)	71 (75)	13 (10)	14.4	3120	1970	>1000
8	28.2 (30)	58.9 (60)	12.9 (10)	19.8	3970	2660	>1000
9	43.6 (45)	44 (45)	12.4 (10)	19.3	3550	2590	>1000
10	55.9 (60)	33.7 (30)	10.4 (10)	20.6	3550	2770	>1000
11	72.4 (75)	16.7 (15)	10.9 (10)	21.6	3300	2890	>1000
12	90.1 (90)	0 (0)	9.9 (10)	19.5	2630	2630	>1000

a) The values of mol. % of TMS-HEMA, Boc-AEMA, EMA (feed compositions) are given in parentheses.

Table S3. Characterization of de-protected copolymers with EMA 20 mol. %

Polymer	HEMA ^a (mol. %)	AEMA ^a (mol. %)	EMA ^a (mol. %)	DP	M_n (NMR) w/TFA	M_n (NMR) w/o TFA	MIC <i>E.coli</i> ($\mu\text{g/mL}$)
13	0 (0)	79.5 (80)	20.5 (20)	17.4	3890	2330	830 ± 290
14	11.8 (10)	67.9 (70)	20.3 (20)	17.9	3770	2390	830 ± 290
15	20.9 (20)	58.6 (60)	20.5 (20)	17.8	3560	2380	1000
16	31 (30)	49.5 (50)	19.5 (20)	18.4	3490	2460	1000
17	39.5 (40)	40.7 (40)	19.8 (20)	15.9	2870	2140	1000
18	49.7 (50)	32.1 (30)	18.2 (20)	18.2	3100	2440	1000

19	59 (60)	22.4 (20)	18.6 (20)	20.6	3260	2740	1000
20	68.9 (70)	13.8 (10)	17.3 (20)	19.1	2850	2550	> 1000
21	82.3 (80)	0 (0)	17.7 (20)	28	4320	3760	> 1000

a) The values of mol. % of TMS-HEMA, Boc-AEMA, EMA (feed compositions) are given in parentheses.

Table S4. Characterization of de-protected copolymers with EMA 30 mol. %

Polymer	HEMA ^a (mol. %)	AEMA ^a (mol. %)	EMA ^a (mol. %)	DP	M_n (NMR) w/TFA	M_n (NMR) w/o TFA	MIC <i>E.coli</i> (μ g/mL)
22	0 (0)	68.9 (70)	31.1 (30)	16.1	3390	2140	250
23	9.2 (7)	59.5 (63)	31.3 (30)	16.4	3280	2170	250
24	14.9 (14)	53.2 (56)	31.9 (30)	17.5	3360	2310	250
25	20.5 (21)	46.8 (49)	32.7 (30)	17.9	3300	2360	250
26	27 (28)	41.3 (42)	31.7 (30)	18.4	3280	2420	250
27	32.3 (35)	34.6 (35)	33.1 (30)	19.1	3250	2510	210 ± 72
28	38.5 (42)	28.6 (28)	32.9 (30)	19	3110	2490	125
29	47.8 (49)	18.4 (21)	33.8 (30)	21.3	3220	2780	250
30	56.2 (56)	10.8 (14)	33 (30)	20.1	2880	2630	500
31	61.7 (63)	6.1 (7)	32.2 (30)	21.2	2920	2770	>1000
32	62.3 (70)	0 (0)	37.7 (30)	11.7	1570	1570	>1000

a) The values of mol. % of TMS-HEMA, Boc-AEMA, EMA (feed compositions) are given in parentheses.

Table S5. Characterization of de-protected copolymers with EMA 40 mol. %

Polymer	HEMA ^a (mol. %)	AEMA ^a (mol. %)	EMA ^a (mol. %)	DP	M_n (NMR) w/TFA	M_n (NMR) w/o TFA	MIC <i>E.coli</i> (μ g/mL)	HC_{50} (μ g/mL)
33	0 (0)	60.1 (60)	39.9 (40)	14.51	2900	1920	31	1000
34	11.9 (10)	50.7 (50)	37.4 (40)	14.44	2740	1910	31	1000
35	21.4 (20)	42.5 (40)	36.1 (40)	15.56	2800	2060	42 ± 18	1000
36	29 (30)	34.1 (30)	36.9 (40)	18.87	3190	2470	31	1000
37	39.8 (40)	23.3 (20)	36.9 (40)	14.78	2350	1960	63	(41% at 1000 μ g/mL)
38	40.3 (50)	13.4 (10)	46.3 (40)	13.25	1950	1750	1000	(5% at 1000 μ g/mL)
39	57.7 (60)	0 (0)	42.3 (40)	12.53	1670	1670	>1000	(5% at 1000 μ g/mL)

a) The values of mol. % of TMS-HEMA, Boc-AEMA, EMA (feed compositions) are given in parentheses.

Table S6. Characterization of de-protected copolymers with EMA 50 mol. %

Polymer	HEMA ^a (mol. %)	AEMA ^a (mol. %)	EMA ^a (mol. %)	DP	M_n (NMR) w/TFA	M_n (NMR) w/o TFA	MIC E.coli (μ g/mL)	HC_{50} (μ g/mL)
40	0 (0)	49.1 (50)	50.9 (50)	19.4	3560	2490	15.62	19 ± 8.2
41	8.1 (7.5)	44.7 (42.5)	47.2 (50)	19.6	3510	2520	15.62	28 ± 8.8
42	14.9 (15)	38.1 (35)	47 (50)	20.06	3440	2580	15.62	28 ± 11
43	21.7 (23)	32.3 (50)	46 (50)	23.9	3930	3060	13 ± 4.5	42 ± 16
44	30.1 (30)	23.6 (20)	46.3 (50)	25.2	3890	3210	26 ± 9.0	94 ± 32
45	39.6 (37.5)	16.7 (12.5)	43.7 (50)	25.1	3690	3210	125	309 ± 32
46	45.3 (45)	8.1 (5)	46.6 (50)	14.2	1990	1860	>1000	7.5 ± 6.9
47	49.7 (50)	0 (0)	50.3 (50)	16.1	2090	2090	>1000	4.7 ± 3.9

a) The values of mol. % of TMS-HEMA, Boc-AEMA, EMA (feed compositions) are given in parentheses.