Synthesis, Structure, Surface and Antimicrobial Properties of New Oligomeric Quaternary Ammonium Salts with Aromatic Spacer

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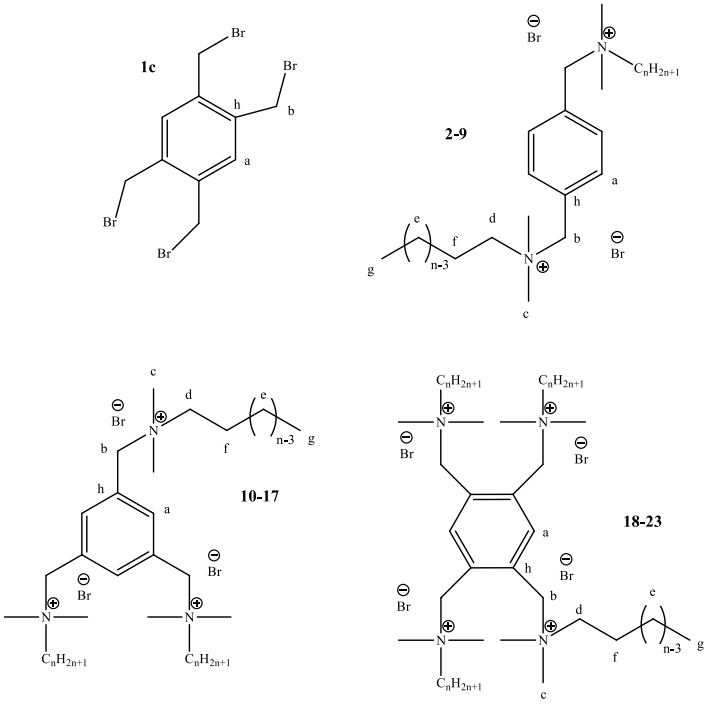
Table S1. Experimental data of synthesized di- tri- and tetrameric alkylammonium surfactants with aromatic spacer and with different chain lengths.

Compound	Molar mass [g/mol]	Reaction Time [h]	Yield [%]	Melting point [°C]	Molecular formula	% N		% C		% H	
						AE	calc.	AE	calc.	AE	calc.
2	466,35	4	90	201-203	$C_{20}H_{38}N_2Br_2$	5,93	5,93	50,43	50,96	8,44	9,39
3	522,45	6	80	206-207	$C_{24}H_{46}N_2Br_2$ x 0,5 H_2O	5,34	5,27	54,19	54,24	9,12	8,91
4	578,56	8	90	210-211	$C_{28}H_{54}N_2Br_2$	4,99	4,84	58,26	58,13	9,60	9,41
5	634,67	8	90	216-217	$C_{32}H_{62}N_2Br_2$	4,54	4,41	60,33	60,56	10,03	9,85
6	690,78	9	95	219-220	$C_{36}H_{70}N_2Br_2$	4,28	4,06	62,34	62,61	10,39	10,21
7	746,89	9	95	221-222	$C_{40}H_{78}N_2Br_2$	3,66	3,75	64,22	64,33	10,69	10,53
8	802,99	10	90	223-224	$C_{44}H_{86}N_2Br_2$	3,56	3,49	65,76	65,81	10,98	10,79
9	859,1	10	90	224-225	$C_{48}H_{94}N_2Br_2$	3,40	3,26	67,43	67,11	11,26	11,03
10	660,46	4	50	218-219	$C_{27}H_{54}N_3Br_3$ x H_2O	5,76	6,19	47,33	47,80	8,53	8,32
11	744,62	6	50	221-222	$C_{33}H_{66}N_3Br_3$ x 1,5 H_2O	5,25	5,45	51,64	51,37	9,22	9,01

12	828,79	7	60	223-224	$C_{39}H_{78}N_3Br_3 \times H_2O$	4,69	4,96	55,41	55,32	9,78	9,52
13	912,95	8	40	225-226	$C_{45}H_{90}N_3Br_3 \times H_2O$	4,28	4,51	58,39	58,06	10,14	9,96
14	997,11	10	70	227-228	$C_{51}H_{102}N_3Br_3 \times 2\ H_2O$	4,03	4,07	59,06	59,29	10,38	10,34
15	1081,27	12	60	229-230	$C_{57}H_{114}N_3Br_3 \times 2\ H_2O$	3,63	3,76	61,01	61,28	10,59	10,64
16	1165,43	13	50	232-234	$C_{63}H_{126}N_3Br_3 \times 1{,}5\ H_2O$	3,34	3,52	64,20	63,46	11,10	10,90
17	1249,6	15	85	235-236	$C_{69}H_{138}N_3Br_3 \times H_2O$	3,23	3,31	65,45	65,38	11,29	11,13
18	966,79	7	15	217-219	$C_{42}H_{86}N_4Br_4 \times H_2O$	5,51	5,69	51,36	51,22	9,34	9,01
19	1079,01	9	5	220-221	$C_{50}H_{102}N_4Br_4 \times 2\ H_2O$	4,69	5,02	54,69	53,86	9,83	9,58
20	1191,22	10	30	221-223	$C_{58}H_{118}N_4Br_4 \times H_2O$	4,47	4,63	57,34	57,61	10,05	10,00
21	1303,44	12	70	224-226	$C_{66}H_{134}N_4Br_4 \times 2\ H_2O$	4,24	4,18	59,22	59,18	10,52	10,38
22	1415,63	13	50	225-226	$C_{74}H_{150}N_4Br_4 \times H_2O$	4,13	3,91	61,65	62,00	10,62	10,69
23	1527,84	14	62	228-230	$C_{82}H_{166}N_4Br_4 \times H_2O$	3,73	3,62	63,46	63,71	10,73	10,95

Table S2. The ^{1}H NMR chemical shifts (ppm) of compounds **1c-10**.



The structures and numbering protons and carbons of compounds **1c-23**.

Protons	1c[b]	2[a]	3[a]	3[b]	4[a]	4[b]	5[a]	5[b]	6[a]	6[b]	7[a]	8[a]	9[a]	10[a]	10[b]
a	7.37	7.76	7.76	7.86	7.75	7.84	7.75	7.84	7.75	7.82	7.75	7.75	7.74	8.09	8.01
b	4.60	4.66	4.66	5.28	4.64	5.29	4.65	5.29	4.64	5.28	4.64	4.64	4.64	4.73	4.83
c	-	3.11	3.11	3.27	3.10	3.26	3.10	3.26	3.10	3.25	3.10	3.09	3.10	3.22	3.11
d	-	3.43	3.41	3.61	3.40	3.60	3.40	3.60	3.39	3.59	3.40	3.38	3.38	3.54	3.42
e	-	1.46	1.41	1.37	1.33, 1.41	1.37, 1.27	1.30, 1.41	1.37, 1.26	1.28, 1.42	1.26, 1.37	1.29, 1.42	1.28, 1.41	1.28, 1.42	1.43	1.42
f	-	1.90	1.91	1.86	1.91	1.86	1.92	1.86	1.91	1.85	1.91	1.91	1.91	1.89	1.92
g	-	1.05	0.94	0.88	0.91	0.88	0.90	0.88	0.90	0.88	0.90	0.89	0.90	1.04	0.94
h	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

[a] in CD_3OD as solvent; [b] in $CDCl_3$ as solvent

Table S3. The ^{1}H NMR chemical shifts (ppm) of compounds **11-23**.

Protons	**11**[a]	**11**[b]	**12**[b]	**13**[b]	**14**[a]	**14**[b]	**15**[b]	**16**[b]	**17**[a]	**18**[b]	**19**[b]	**20**[b]	**21**[a]	**21**[b]	**22**[b]	**23**[b]
a	8.09	8.06	8.03	8.01	8.07	8.00	8.00	8.00	8.07	8.19	8.11	8.09	8.27	8.04	8.24	8.14
b	4.74	4.93	5,00	4.99	4.73	5.01	5.00	5.04	4.72	5.22	5.21	5.17	5.08	5.15	5.23	5.13
c	3.22	3.27	3.30	3.29	3.22	3.29	3.29	3.29	3.22	3.34	3.34	3.35	3.19	3.37	3.35	3.36
d	3.54	3.63	3.64	3.63	3.53	3.63	3.63	3.62	3.53	4.06	4.09	4.10	3.78	4.12	4.07	4.10
e	1.45	1.34	1.25, 1.34	1.25, 1.35	1.30, 1.41	1.34, 1.25	1.25, 1.34	1.25, 1.32	1.29	1.39	1.41	1.27, 1.40	1.30, 1.45	1.27, 1.40	1.39, 1.45	1.26, 1.40
f	1.90	1.80	1.79	1.78	1.90	1.78	1.79	1.78	1.91	1.83	1.83	1.82	1.93	1.79	1.82	1.81
g	1.04	0.88, 0.90	0.87	0.88	0.90	0.88	0.88	0.88	0.90	0.91	0.89	0.89	0.90	0.89	0.88	0.88
h	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

[a] in CD_3OD as solvent; [b] in $CDCl_3$ as solvent

Table S4. The ^{13}C NMR chemical shifts (ppm) of compounds **1c-10**.

Carbon	**1c**[b]	**2**[a]	**3**[a]	**3**[b]	**4**[a]	**4**[b]	**5**[a]	**5**[b]	**6**[a]	**6**[b]	**7**[a]	**8**[a]	**9**[a]	**10**[a]	**10**[b]
a	137.6	135.0	135.0	133.9	135.0	134.0	135.0	134.0	135.0	134.0	135.0	135.0	135.0	141.2	139.6
b	28.7	66.0	66.1	64.5	66.2	64.7	66.2	64.7	66.2	64.8	66.2	66.1	66.0	66.1	64.5
c	-	50.6	50.6	49.3	50.6	49.4	50.6	49.3	50.6	49.4	50.5	50.6	50.6	50.6	49.1
d	-	67.9	67.9	66.1	67.9	65.9	67.9	66.0	67.9	66.0	68.0	68.1	67.8	68.0	66.7
e, f	-	25.7, 20.8	32.5, 23.6, 23.7, 27.2	31.1, 26.0, 22.8, 22.3	32.9, 30.3, 27.5, 23.8, 23.7	31.5, 29.2, 29.0, 26.3, 22.9, 22.5	33.1, 30.7, 30.4, 27.5, 23.8	31.7, 29.3, 29.2, 29.1, 26.3, 22.9, 22.5	33.1, 30.8, 30.7, 30.5, 30.4, 27.5, 23.8	31.8, 29.5, 29.4, 29.3, 26.4, 23.0, 22.6	33.1, 30.8, 30.7, 30.6, 30.5, 30.4, 27.5, 23.8	33.1, 30.8, 30.7, 30.6, 30.5, 30.4, 27.5, 23.8	33.1, 30.8, 30.7, 30.5, 30.4, 27.5, 23.8	25.7, 20.9	24.4, 19.5
g	-	14.0	14.3	13.8	14.5	13.9	14.5	13.9	14.5	14.0	14.5	14.6	14.5	14.1	13.5

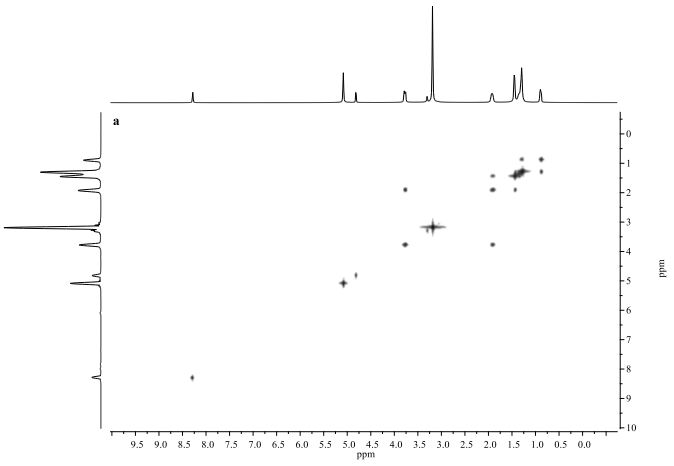
h	133.6	131.6	131.6	130.0	131.6	130.0	131.6	130.0	131.6	130.0	131.6	131.6	131.6	131.3	129.3

[a] in CD_3OD as solvent; [b] in $CDCl_3$ as solvent

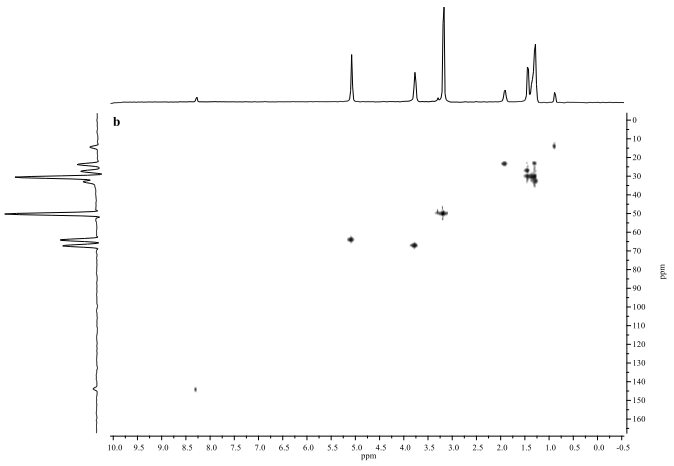
Table S5. The ^{13}C NMR chemical shifts (ppm) of compounds **11-23**.

Carbon	**11**[a]	**11**[b]	**12**[b]	**13**[b]	**14**[a]	**14**[b]	**15**[b]	**16**[b]	**17**[a]	**18**[b]	**19**[b]	**20**[b]	**21**[a]	**21**[b]	**22**[b]	**23**[b]
a	141.2	140	139.8	139.8	141.2	139.8	139.9	139.8	141.2	142.0	142.0	141.9	146.3	141.7	142.2	141.8
b	66.3	64.5	64.4	64.5	66.2	64.6	64.6	64.4	66.0	62.4	62.5	62.6	66.7	62.6	62.5	62.4
c	50.6	49.4	49.3	49.3	50.6	49.4	49.4	49.4	50.6	49.9	49.9	49.9	52.8	50.0	49.8	49.8
d	68.0	66.9	67.1	67.1	68.2	67.2	67.2	67.3	68.2	65.7	65.8	65.9	69.8	65.9	65.8	66.0
e, f	32.5, 27.2, 23.7, 23.6	31.3, 25.9, 22.7, 22.4	31.7, 29.2, 29.0, 26.2, 22.7, 22.5	31.8, 29.5, 29.4, 29.3, 29.2, 26.2, 22.7, 22.5	33.1, 30.8, 30.7, 30.5, 27.6, 23.8	31.8, 29.6, 29.4, 29.3, 22.8, 22.6	31.9, 29.6, 29.5, 29.3, 26.3, 22.8, 22.6	31.9, 29.7, 29.6, 29.5, 29.4, 29.3, 26.2, 25.9, 22.8, 22.6	33.2, 30.9, 30.8, 30.7, 30.6, 30.5, 27.6, 26.7, 23.8	31.4, 26.0, 23.0, 22.4	31.6, 27.5, 26.0, 23.4, 22.7	31.7, 29.2, 27.4, 26.4, 23.2, 22.6	35.6, 33.3, 33.2, 33.0, 30.0, 26.5, 26.3	31.9, 29.6, 29.5, 29.3, 26.4, 23.2, 22.6	29.7, 29.6, 29.5, 29.4, 27.1, 26.5, 25.7, 23.2, 22.7	31.9, 29.7, 29.6, 29.5, 29.3, 26.4
g	14.4	14.0	14.0	14.0	14.5	14.0	14.1	14.1	14.5	13.9	13.9	14.0	17.0	14.1	14.1	14.1
h	131.3	129.3	129.2	129.2	131.3	129.3	129.3	129.3	131.3	132.4	132.7	132.5	136.5	132.5	132.6	132.5

[a] in CD_3OD as solvent; [b] in $CDCl_3$ as solvent



a)



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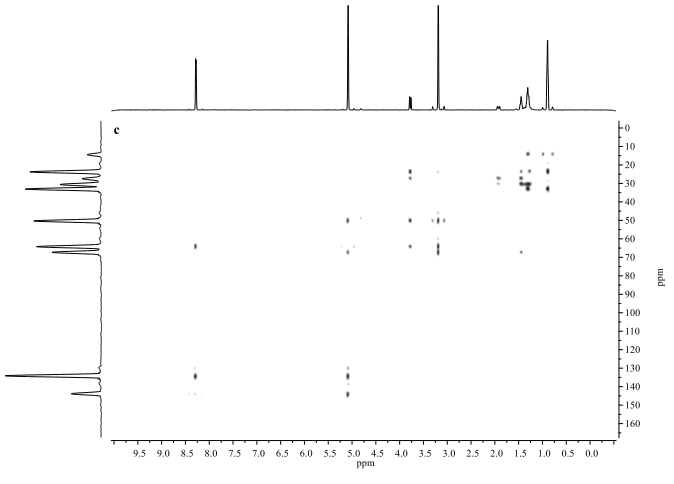

c)

Figure S1. 2D NMR spectra of compound **21**: COSY (a), HSQC (b) and HMBC (c).

Synthesis:

Synthesis*1,4-di-[N-(1-butyl)-N,N-dimethylammoniummethyl)benzene dibromide* (**2**) RT = 4 h, white solid (90%), m. p. 201-203 °C. ^{1}H NMR (CD_3OD) δ: 7.76 ppm (4H, a), 4.66 ppm (4H, b), 3.43 ppm (4H, d), 3.11 ppm (12H, c), 1.90 ppm (4H, f), 1.46 ppm (4H, e), 1.05 ppm (6H, g). ^{13}C NMR (CD_3OD) δ: 135.0 ppm (a), 131.6 ppm (h), 67.9 ppm (d), 66.0 ppm (b), 50.6 ppm (c), 25.7 and 20.8 ppm (e,f), 14.0 ppm (g). Elemental analysis for $C_{20}H_{38}N_2Br_2$ found (calc.): %N 5.93 (5.93); %C 50.43 (50.96); %H 8.44 (9.39). ESI(+)-MS (*m*/*z*): 153.1 ($C_{20}H_{38}N_2$/2). FT-IR (KBr) ν_{max}: 3503, 3014, 2967, 2874, 1618, 1489, 1384, 1221, 1011, 942, 884, 826, 733.

1,4-di-[N-(1-hexyl)-N,N-dimethylammoniummethyl)benzene dibromide (**3**) RT = 6 h, white solid (80%), m. p. 206-207 °C. ^{1}H NMR (CD_3OD) δ: 7.76 ppm (4H, a), 4.66 ppm (4H, b), 3.41 ppm (4H, d), 3.11 ppm (12H, c), 1.91 ppm (4H, f), 1.41 ppm (12H, e), 0.94 ppm (6H, g). ^{1}H NMR ($CDCl_3$) δ: 7.86 ppm (4H, a), 5.28 ppm (4H, b), 3.61 ppm (4H, d), 3.27 ppm (12H, c), 1.86 ppm (4H, f), 1.37 ppm (12H, e), 0.88 ppm (6H, g). ^{13}C NMR (CD_3OD) δ: 135.0 ppm (a), 131.6 ppm (h), 67.9 ppm (d), 66.1 ppm (b), 50.6 ppm (c), 32.5, 27.2, 23.7 and 23.6 ppm (e,f), 14.3 ppm (g). ^{13}C NMR ($CDCl_3$) δ: 133.9 ppm (a), 130.0 ppm (h), 66.1 ppm (d), 64.5 ppm (b), 49.3 ppm (c), 31.1, 26.0, 22.8 and 22.3 ppm (e,f), 13.8 ppm (g). Elemental analysis for $C_{24}H_{46}N_2Br_2 \cdot 0.5\ H_2O$ found (calc.): %N 5.34 (5.27); %C 54.19 (54.24); %H 9.12 (8.91). ESI(+)-MS (*m*/*z*): 181.2 ($C_{24}H_{46}N_2$/2).

1,4-di-[N,N-dimethyl-N-(1-octyl)ammoniummethyl)benzene dibromide (**4**) RT = 8 h, white solid (90%), m. p. 210-211 °C. ^{1}H NMR (CD_3OD) δ: 7.75 ppm (4H, a), 4.64 ppm (4H, b), 3.40 ppm (4H, d), 3.10 ppm (12H, c), 1.91 ppm (4H, f), 1.41 and 1.33 ppm (20H, e), 0.91 ppm (6H, g). ^{1}H NMR ($CDCl_3$) δ: 7.84 ppm (4H, a), 5.29 ppm (4H, b), 3.60 ppm (4H, d), 3.26 ppm (12H, c), 1.86 ppm (4H, f), 1.27, 1.37 ppm (20H, e), 0.88 ppm (6H, g). ^{13}C NMR (CD_3OD) δ: 135.0 ppm (a), 131.6 ppm (h), 67.9 ppm (d), 66.2 ppm (b), 50.6 ppm (c), 32.9, 30.3, 27.5, 23.7 and 23.7 ppm (e,f), 14.5 ppm (g). ^{13}C NMR ($CDCl_3$) δ: 134.0 ppm (a), 130.0 ppm (h), 65.9 ppm (d), 64.7 ppm (b), 49.4 ppm (c), 31.5, 29.2, 29.0, 26.3, 22.9 and 22.5 ppm (e,f), 13.9 ppm (g). Elemental analysis for $C_{28}H_{54}N_2Br_2$ found (calc.): %N 4.99 (4.84); %C 58.26 (58.13); %H 9.60 (9.41). ESI(+)-MS (*m*/*z*): 209.2 ($C_{28}H_{54}N_2$/2).

1,4-di-[N-(1-decyl)-N,N-dimethylammoniummethyl)benzene dibromide (**5**) RT = 8 h, white solid (90%), m. p. 216-217 °C. ^{1}H NMR (CD_3OD) δ: 7.75 ppm (4H, a), 4.65 ppm (4H, b), 3.40 ppm (4H, d), 3.10 ppm (12H,

c), 1.92 ppm (4H, f), 1.41 and 1.30 ppm (28H, e), 0.90 ppm (6H, g). ^{1}H NMR ($CDCl_3$) δ: 7.84 ppm (4H, a), 5.29 ppm (4H, b), 3.60 ppm (4H, d), 3.26 ppm (12H, c), 1.86 ppm (4H, f), 1.37 and 1.26 ppm (28H, e), 0.88 ppm (6H, g). ^{13}C NMR (CD_3OD) δ: 135.0 ppm (a), 131.6 ppm (h), 67.9 ppm (d), 66.2 ppm (b), 50.6 ppm (c), 33.1, 30.7, 30.4, 27.5 and 23.8 ppm (e,f), 14.5 ppm (g). ^{13}C NMR ($CDCl_3$) δ: 134.0 ppm (a), 130.0 ppm (h), 66.0 ppm (d), 64.7 ppm (b), 49.3 ppm (c), 31.7, 29.3, 29.2, 29.1, 26.3, 22.9 and 22.5 ppm (e,f), 13.9 ppm (g). Elemental analysis for $C_{32}H_{62}N_2Br_2$ found (calc.): %N 4.54 (4.41); %C 60.33 (60.56); %H 10.03 (9.85). ESI(+)-MS (*m*/*z*): 237.2 ($C_{32}H_{62}N_2$/2).

1,4-di-[N-(1-dodecyl)-N,N-dimethylammoniummethyl)benzene dibromide (**6**) RT = 9 h, white solid (95%), m. p. 219-220 °C. ^{1}H NMR (CD_3OD) δ: 7.75 ppm (4H, a), 4.64 ppm (4H, b), 3.39 ppm (4H, d), 3.10 ppm (12H, c), 1.91 ppm (4H, f), 1.42 and 1.28 ppm (36H, e), 0.90 ppm (6H, g). ^{1}H NMR ($CDCl_3$) δ: 7.82 ppm (4H, a), 5.28 ppm (4H, b), 3.59 ppm (4H, d), 3.25 ppm (12H, c), 1.85 ppm (4H, f), 1.37 and 1.26 ppm (36H, e), 0.88 ppm (6H, g). ^{13}C NMR (CD_3OD) δ: 135.0 ppm (a), 131.6 ppm (h), 67.9 ppm (d), 66.2 ppm (b), 50.6 ppm (c), 33.1, 30.8, 30.7, 30.5, 30.4, 27.5 and 23.8 ppm (e,f), 14.5 ppm (g). ^{13}C NMR ($CDCl_3$) δ: 134.0 ppm (a), 130.0 ppm (h), 66.0 ppm (d), 64.8 ppm (b), 49.4 ppm (c), 31.8, 29.5, 29.4, 29.3, 26.4, 23.0 and 22.6 ppm (e,f), 14.0 ppm (g). Elemental analysis for $C_{36}H_{70}N_2Br_2$ found (calc.): %N 4.28 (4.06); %C 62.34 (62.61); %H 10.39 (10.21). ESI(+)-MS (*m*/*z*): 265.7 ($C_{36}H_{70}N_2$/2). FT-IR (KBr) ν_{max}: 3402, 3009, 2959, 2918, 2854, 1490, 1456, 1430, 1219, 1005, 880, 824, 721.

1,4-di-[N,N-dimethyl-N-(1-tetradecyl)ammoniummethyl)benzene dibromide (**7**) RT = 9 h, white solid (95%), m. p. 221-222 °C. ^{1}H NMR (CD_3OD) δ: 7.75 ppm (4H, a), 4.64 ppm (4H, b), 3.40 ppm (4H, d), 3.10 ppm (12H, c), 1.91 ppm (4H, f), 1.42 and 1.29 ppm (44H, e), 0.90 ppm (6H, g). ^{13}C NMR (CD_3OD) δ: 135.0 ppm (a), 131.6 ppm (h), 68.0 ppm (d), 66.2 ppm (b), 50.5 ppm (c), 33.1, 30.8, 30.7, 30.6, 30.5, 30.4, 27.5 and 23.8 ppm (e,f), 14.5 ppm (g). Elemental analysis for $C_{40}H_{78}N_2Br_2$ found (calc.): %N 3.66 (3.75); %C 64.22 (64.33); %H 10.69 (10.53). ESI(+)-MS (*m*/*z*): 293.5 ($C_{40}H_{78}N_2$/2).

1,4-di-[N-(1-hexadecyl)-N,N-dimethylammoniummethyl)benzene dibromide (**8**) RT = 10 h, white solid (90%), m. p. 223-224 °C. ^{1}H NMR (CD_3OD) δ: 7.75 ppm (4H, a), 4.64 ppm (4H, b), 3.38 ppm (4H, d), 3.09 ppm (12H, c), 1.91 ppm (4H, f), 1.41 and 1.28 ppm (52H, e), 0.89 ppm (6H, g). ^{13}C NMR (CD_3OD) δ: 135.0 ppm (a), 131.6 ppm (h), 68.1 ppm (d), 66.1 ppm (b), 50.6 ppm (c), 33.1, 30.8, 30.7, 30.6, 30.5, 30.4, 27.5 and 23.8 ppm (e,f), 14.6 ppm (g). Elemental analysis for $C_{44}H_{86}N_2Br_2$ found (calc.): %N 3.56 (3.49); %C 65.76 (65.81); %H 10.98 (10.79). ESI(+)-MS (*m*/*z*): 321.6 ($C_{44}H_{86}N_2$/2).

1,4-di-[N,N-dimethyl-N-(1-octadecyl)ammoniummethyl)benzene dibromide (**9**) RT = 10 h, white solid (90%), m. p. 224-225 °C. ^{1}H NMR (CD_3OD) δ: 7.74 ppm (4H, a), 4.64 ppm (4H, b), 3.38 ppm (4H, d), 3.10 ppm (12H, c), 1.91 ppm (4H, f), 1.42 and 1.28 ppm (60H, e), 0.90 ppm (6H, g). ^{13}C NMR (CD_3OD) δ: 135.0 ppm (a), 131.6 ppm (h), 67.8 ppm (d), 66.0 ppm (b), 50.6 ppm (c), 33.1, 30.8, 30.7, 30.6, 30.5, 30.4, 27.5 and 23.8 ppm (e,f), 14.5 ppm (g). Elemental analysis for $C_{48}H_{94}N_2Br_2$ found (calc.): %N 3.40 (3.26); %C 67.43 (67.11); %H 11.26 (11.03). ESI(+)-MS (*m*/*z*): 349.8 ($C_{48}H_{94}N_2$/2). FT-IR (KBr) ν_{max}: 3383, 3025, 2921, 2851, 1487, 1420, 1384, 1221, 1011, 872, 826, 722.

1,3,5-tris-[N-(1-butyl)-N,N-dimethylammoniummethyl)benzene tribromide (**10**) RT = 4 h, white solid (50%), m. p. 218-219 °C. ^{1}H NMR (CD_3OD) δ: 8.09 ppm (3H, a), 4.73 ppm (6H, b), 3.54 ppm (6H, d), 3.22 ppm (18H, c), 1.89 ppm (6H, f), 1.43 ppm (6H, e), 1.04 ppm (9H, g). ^{1}H NMR ($CDCl_3$) : 8.01 ppm (3H, a), 4.83 ppm (6H, b), 3.42 ppm (6H, d), 3.11 ppm (18H, c), 1.81 ppm (6H, f), 1.42 ppm (6H, e), 0.94 ppm (9H, g). ^{13}C NMR (CD_3OD) δ: 141.2 ppm (a), 131.3 ppm (h), 68.0 ppm (d), 66.1 ppm (b), 50.6 ppm (c), 25.7 and 20.9 ppm (e,f), 14.1 ppm (g). ^{13}C NMR ($CDCl_3$) δ: 139.6 ppm (a), 129.3 ppm (h), 66.7 ppm (d), 64.5 ppm (b), 49.1 ppm (c), 24.4 ppm (f), 19.5 ppm (e), 13.5 ppm (g). Elemental analysis for $C_{27}H_{54}N_3Br_3 \cdot H_2O$ found (calc.): %N 5.76 (6.19); %C 47.33 (47.80); %H 8.53 (8.32). ESI(+)-MS (*m*/*z*): 140.2 ($C_{27}H_{54}N_3$/3). FT-IR (KBr) ν_{max}: 3434, 3014, 2983, 2878, 2076, 1642, 1488, 1454, 1384, 1190, 1038, 882, 754.

1,3,5-tris-[N-(1-hexyl)-N,N-dimethylammoniummethyl)benzene tribromide (**11**) RT = 6 h, white solid (50%), m. p. 221-222 °C. ^{1}H NMR (CD_3OD) δ: 8.09 ppm (3H, a), 4.74 ppm (6H, b), 3.54 ppm (6H, d), 3.22 ppm (18H, c), 1.90 ppm (6H, f), 1.45 ppm (18H, e), 1.04 ppm (9H, g). ^{1}H NMR ($CDCl_3$): 8.06 ppm (3H, a), 4.93 ppm (6H, b), 3.63 ppm (6H, d), 3.27 ppm (18H, c), 1.80 ppm (6H, f), 1.34 ppm (18H, e), 0.90 and 0.88 ppm (9H, g). ^{13}C NMR (CD_3OD) δ: 141.2 ppm (a), 131.3 ppm (h), 68.0 ppm (d), 66.3 ppm (b), 50.6 ppm (c), 32.5, 27.2, 23.7 and 23.6 ppm (e,f), 14.4 ppm (g). ^{13}C NMR ($CDCl_3$) δ: 140.0 ppm (a), 129.3 ppm (h), 66.9 ppm (d), 64.5 ppm (b), 49.4 ppm (c), 31.3, 29.9, 22.7 and 22.4 ppm (e, f), 14.0 ppm (g). Elemental analysis for $C_{33}H_{66}N_3Br_3 \cdot 1.5\ H_2O$ found (calc.): %N 5.25 (5.45); %C 51.64 (51.37); %H 9.22 (9.01). ESI(+)-MS (*m*/*z*): 168.3 ($C_{33}H_{66}N_3/3$).

1,3,5-tris-[N,N-dimethyl-N-(1-octyl)ammoniummethyl)benzene tribromide (**12**) RT = 7 h, white solid (60%), m. p. 223-224 °C. ^{1}H NMR ($CDCl_3$) δ: 8.03 ppm (3H, a), 5.00 ppm (6H, b), 3.64 ppm (6H, d), 3.30 ppm (18H, c), 1.79 ppm (6H, f), 1.34 and 1.25 ppm (30H, e), 0.87 ppm (9H, g). ^{13}C NMR ($CDCl_3$) δ: 139.8 ppm (a), 129.2 ppm (h), 67.1 ppm (d), 64.4 ppm (b), 49.3 ppm (c), 31.7, 29.2, 29.0, 26.2, 22.7 and 22.5 ppm (e,f), 14.0 ppm (g). Elemental analysis for $C_{39}H_{78}N_3Br_3 \cdot H_2O$ found (calc.): %N 4.69 (4.96); %C 55.41 (55.32); %H 9.78 (9.52). ESI(+)-MS (*m*/*z*): 196.4 ($C_{39}H_{78}N_3/3$).

1,3,5-tris-[N-(1-decyl)-N,N-dimethylammoniummethyl)benzene tribromide (**13**) RT = 8 h, white solid (40%), m. p. 225-226 °C. ^{1}H NMR ($CDCl_3$) δ: 8.01 ppm (3H, a), 4.99 ppm (6H, b), 3.63 ppm (6H, d), 3.29 ppm (18H, c), 1.78 ppm (6H, f), 1.35 and 1.25 ppm (42H, e), 0.88 ppm (9H, g). ^{13}C NMR ($CDCl_3$) δ: 139.8 ppm (a), 129.9 ppm (h), 67.1 ppm (d), 64.5 ppm (b), 49.3 ppm (c), 31.8, 29.5, 29.4, 29.3, 29.2, 26.2, 22.7 and 22.5 ppm (e,f), 14.0 ppm (g). Elemental analysis for $C_{45}H_{90}N_3Br_3 \cdot H_2O$ found (calc.): %N 4.28 (4.51); %C 58.39 (58.06); %H 10.14 (9.96). ESI(+)-MS (*m*/*z*): 224.2 ($C_{45}H_{90}N_3/3$).

1,3,5-tris-[N-(1-dodecyl)-N,N-dimethylammoniummethyl)benzene tribromide (**14**) RT = 10 h, white solid (70%), m. p. 227-228 °C. ^{1}H NMR (CD_3OD) δ: 8.07 ppm (3H, a), 4.73 ppm (6H, b), 3.53 ppm (6H, d), 3.22 ppm (18H, c), 1.90 ppm (6H, f), 1.41 and 1.30 ppm (54H, e), 0.90 ppm (9H, g). ^{1}H NMR ($CDCl_3$) δ: 8.00 ppm (3H, a), 5.01 ppm (6H, b), 3.63 ppm (6H, d), 3.29 ppm (18H, c), 1.78 ppm (6H, f), 1.34 and 1.25 ppm (54H, e), 0.88 ppm (9H, g). ^{13}C NMR (CD_3OD) δ: 141.2 ppm (a), 131.3 ppm (h), 68.2 ppm (d), 66.2 ppm (b), 50.6 ppm (c), 33.1, 30.8, 30.7, 30.5, 27.6 and 23.8 ppm (e,f), 14.5 ppm (g). ^{13}C NMR ($CDCl_3$) δ: 139.8 ppm (a), 129.3 ppm (h), 67.2 ppm (d), 64.6 ppm (b), 49.4 ppm (c), 31.8, 29.6, 29.4, 29.3, 22.8 and 22.6 ppm (e,f), 14.0 ppm (g). Elemental analysis for $C_{51}H_{102}N_3Br_3 \cdot 2\ H_2O$ found (calc.): %N 4.03 (4.07); %C 59.06 (59.29); %H 10.38 (10.34). ESI(+)-MS (*m*/*z*): 252.5 ($C_{51}H_{102}N_3/3$). FT-IR (KBr) ν_{max}: 3437, 3018, 2928, 2854, 1755, 1490, 1468, 1436, 1381, 1195, 1033, 753, 724.

1,3,5-tris-[N,N-dimethyl-N-(1-tetradecyl)ammoniummethyl)benzene tribromide (**15**) RT = 12 h, white solid (60%), m. p. 229-230 °C. ^{1}H NMR ($CDCl_3$) δ: 8.00 ppm (3H, a), 5.00 ppm (6H, b), 3.63 ppm (6H, d), 3.29 ppm (18H, c), 1.79 ppm (6H, f), 1.34 and 1.25 ppm (66H, e), 0.88 ppm (9H, g). ^{13}C NMR ($CDCl_3$) δ: 139.9 ppm (a), 129.3 ppm (h), 67.2 ppm (d), 64.6 ppm (b), 49.4 ppm (c), 31.9, 29.6, 29.5, 29.3, 26.3, 22.8 and 22.6 ppm (e,f), 14.1 ppm (g). Elemental analysis for $C_{57}H_{114}N_3Br_3 \cdot 2\ H_2O$ found (calc.): %N 3.63 (3.76); %C 61.01 (61.28); %H 10.59 (10.64). ESI(+)-MS (*m*/*z*): 280.5 ($C_{57}H_{114}N_3/3$). FT-IR (KBr) ν_{max}: 3435, 3018, 2920, 2853, 1620, 1489, 1469, 1432, 1373, 1197, 1030, 897, 753, 722, 672.

1,3,5-tris-[N-(1-hexadecyl)-N,N-dimethylammoniummethyl)benzene tribromide (**16**) RT = 13 h, white solid (50%), m. p. 232-234 °C. ^{1}H NMR ($CDCl_3$) δ: 8.00 ppm (3H, a), 5.04 ppm (6H, b), 3.62 ppm (6H, d), 3.29 ppm (18H, c), 1.78 ppm (6H, f), 1.32 and 1.25 ppm (78H, e), 0.88 ppm (9H, g). ^{13}C NMR ($CDCl_3$) δ: 139.8 ppm (a), 129.3 ppm (h), 67.3 ppm (d), 64.4 ppm (b), 49.4 ppm (c), 31.9, 29.7, 29.6, 29.5, 29.4, 29.3, 26.2, 25.9, 22.8 and 22.6 ppm (e,f), 14.1 ppm (g). Elemental analysis for $C_{63}H_{126}N_3Br_3 \cdot 1.5\ H_2O$ found (calc.): %N 3.34 (3.52); %C 64.20 (63.46); %H 11.10 (10.90). ESI(+)-MS (*m*/*z*): 308.6 ($C_{63}H_{126}N_3/3$).

1,3,5-tris-[N,N-dimethyl-N-(1-octadecyl)ammoniummethyl)benzene tribromide (**17**) RT = 15 h, white solid (85%), m. p. 235-236 °C. ^{1}H NMR (CD_3OD) δ: 8.07 ppm (3H, a), 4.72 ppm (6H, b), 3.53 ppm (6H, d),

3.22 ppm (18H, c), 1.91 ppm (6H, f), 1.29 ppm (90H, e), 0.90 ppm (9H, g). ^{13}C NMR (CD_3OD) δ: 141.2 ppm (a), 131.3 ppm (h), 68.2 ppm (d), 66.0 ppm (b), 50.6 ppm (c), 33.2, 30.9, 30.8, 30.7, 30.6, 30.5, 27.6, 26.7 and 23.8 ppm (e,f), 14.5 ppm (g). Elemental analysis for $C_{69}H_{138}N_3Br_3 \cdot H_2O$ found (calc.): %N 3.23 (3.31); %C 65.45 (65.38); %H 11.29 (11.13). ESI(+)-MS (*m*/*z*): 336.6 ($C_{69}H_{138}N_3/3$). FT-IR (KBr) ν_{max}: 3426, 3012, 2921, 2852, 1717, 1625, 1465, 1453, 1373, 1190, 1030, 904, 755, 720.

1,2,4,5-tetrakis-[N-(1-hexyl)-N,N-dimethylammoniummethyl)benzene tetrabromide (**18**) RT = 7 h, white solid (15%), m. p. 217-219 °C. ^{1}H NMR ($CDCl_3$) δ: 8.19 ppm (2H, a), 5.22 ppm (8H, b), 4.06 ppm (8H, d), 3.34 ppm (24H, c), 1.83 ppm (8H, f), 1.39 ppm (24H, e), 0.91 ppm (12H, g). ^{13}C NMR ($CDCl_3$) δ: 142.0 ppm (a), 132.4 ppm (h), 65.7 ppm (d), 62.4 ppm (b), 49.9 ppm (c), 31.4, 26.0, 23.0 and 22.4 ppm (e,f), 13.9 ppm (g). Elemental analysis for $C_{42}H_{86}N_4Br_4 \cdot H_2O$ found (calc.): %N 5.51 (5.69); %C 51.36 (51.22); %H 9.34 (9.01). ESI(+)-MS (*m*/*z*): 161.8 ($C_{42}H_{86}N_4/4$).

1,2,4,5-tetrakis-[N,N-dimethyl-N-(1-octyl)ammoniummethyl)benzene tetrabromide (**19**) RT = 9 h, white solid (5%), m. p. 220-221 °C. ^{1}H NMR ($CDCl_3$) δ: 8.11 ppm (2H, a), 5.21 ppm (8H, b), 4.09 ppm (8H, d), 3.34 ppm (24H, c), 1.83 ppm (8H, f), 1.41 ppm (40H, e), 0.89 ppm (12H, g). ^{13}C NMR ($CDCl_3$) δ: 142.0 ppm (a), 132.7 ppm (h), 65.8 ppm (d), 62.5 ppm (b), 49.9 ppm (c), 31.6, 27.5, 26.0, 23.4 and 22.7 ppm (e,f), 13.9 ppm (g). Elemental analysis for $C_{50}H_{102}N_4Br_4 \cdot 2\ H_2O$ found (calc.): %N 4.69 (5.02); %C 54.69 (53.86); %H 9.83 (9.58). ESI(+)-MS (*m*/*z*): 189.8 ($C_{50}H_{102}N_4/4$).

1,2,4,5-tetrakis-[N-(1-decyl)-N,N-dimethylammoniummethyl)benzene tetrabromide (**20**) RT = 10 h, white solid (30%), m. p. 221-223 °C. ^{1}H NMR ($CDCl_3$) δ: 8.09 ppm (2H, a), 5.17 ppm (8H, b), 4.10 ppm (8H, d), 3.35 ppm (24H, c), 1.82 ppm (8H, f), 1.40 and 1.27 ppm (56H, e), 0.89 ppm (12H, g). ^{13}C NMR ($CDCl_3$) δ: 141.9 ppm (a), 132.5 ppm (h), 65.9 ppm (d), 62.6 ppm (b), 49.9 ppm (c), 31.7, 29.2, 27.4, 26.4, 23.2 and 22.6 ppm (e,f), 14.0 ppm (g). Elemental analysis for $C_{58}H_{118}N_4Br_4 \cdot H_2O$ found (calc.): %N 4.47 (4.63); %C 57.34 (57.61); %H 10.05 (10.00). ESI(+)-MS (*m*/*z*): 217.9 ($C_{58}H_{118}N_4/4$).

1,2,4,5-tetrakis-[N-(1-dodecyl)-N,N-dimethylammoniummethyl)benzene tetrabromide (**21**) RT = 12 h, white solid (70%), m. p. 224-226 °C. ^{1}H NMR (CD_3OD) δ: 8.27 ppm (2H, a), 5.08 ppm (8H, b), 3.78 ppm (8H, d), 3.19 ppm (24H, c), 1.93 ppm (8H, f), 1.45 and 1.30 ppm (72H, e), 0.90 ppm (12H, g). ^{1}H NMR ($CDCl_3$) δ: 8.04 ppm (2H, a), 5.15 ppm (8H, b), 4.12 ppm (8H, d), 3.37 ppm (24H, c), 1.79 ppm (8H, f), 1.40 and 1.27 ppm (72H, e), 0.89 ppm (12H, g). ^{13}C NMR (CD_3OD) δ: 146.3 ppm (a), 136.5 ppm (h), 69.8 ppm (d), 66.7 ppm (b), 52.8 ppm (c), 35.6, 33.3, 33.2, 33.0, 30.0, 26.5 and 26.3 ppm (e,f), 17.0 ppm (g). ^{13}C NMR ($CDCl_3$) δ: 141.7 ppm (a), 132.5 ppm (h), 65.9 ppm (d), 62.6 ppm (b), 50.0 ppm (c), 31.9, 29.6, 29.5, 29.3, 26.4, 23.2 and 22.6 ppm (e,f), 14.1 ppm (g). Elemental analysis for $C_{66}H_{134}N_4Br_4 \cdot 2\ H_2O$ found (calc.): %N 4.24 (4.18); %C 59.22 (59.18); %H 10.52 (10.38). ESI(+)-MS (*m*/*z*): 245.9 ($C_{66}H_{134}N_4/4$). FT-IR (KBr) ν_{max}: 3409, 3020, 2924, 2854, 1620, 1469, 1380, 1235, 1015, 891, 866, 849, 722.

1,2,4,5-tetrakis-[N,N-dimethyl-N-(1-tetradecyl)ammoniummethyl)benzene tetrabromide (**22**) RT = 13 h, white solid (50%), m. p. 225-226 °C. ^{1}H NMR ($CDCl_3$) δ: 8.24 ppm (2H, a), 5.23 ppm (8H, b), 4.07 ppm (8H, d), 3.35 ppm (24H, c), 1.82 ppm (8H, f), 1.45 and 1.39 ppm (88H, e), 0.88 ppm (12H, g). ^{13}C NMR ($CDCl_3$) δ: 142.2 ppm (a), 132.6 ppm (h), 65.8 ppm (d), 62.5 ppm (b), 49.8 ppm (c), 29.7, 29.6, 29.5, 29.4, 27.1, 26.5, 25.7, 23.2 and 22.7 ppm (e,f), 14.1 ppm (g). Elemental analysis for $C_{74}H_{150}N_4Br_4 \cdot H_2O$ found (calc.): %N 4.13 (3.91); %C 61.65 (62.00); %H 10.62 (10.69). ESI(+)-MS (*m*/*z*): 273.9 ($C_{74}H_{150}N_4/4$). FT-IR (KBr) ν_{max}: 3020, 2924, 2854, 1620, 1469, 1380, 1235, 1015, 891, 866, 849, 722.

1,2,4,5-tetrakis-[N-(1-hexadecyl)-N,N-dimethylammoniummethyl)benzene tetrabromide (**23**) RT = 14 h, white solid (62%), m. p. 228-230 °C. ^{1}H NMR ($CDCl_3$) δ: 8.14 ppm (2H, a), 5.14 ppm (8H, b), 4.10 ppm (8H, d), 3.36 ppm (24H, c), 1.81 ppm (8H, f), 1.40 and 1.26 ppm (104H, e), 0.88 ppm (12H, g). ^{13}C NMR ($CDCl_3$) δ: 141.8 ppm (a), 132.5 ppm (h), 66.0 ppm (d), 62.4 ppm (b), 49.8 ppm (c), 31.9, 29.7, 29.6, 29.5, 29.3 and 26.4 ppm (e,f), 14.1 ppm (g). Elemental analysis for $C_{82}H_{166}N_4Br_4 \cdot H_2O$ found (calc.): %N 3.73 (3.62);

%C 63.46 (63.71); %H 10.73 (10.95). ESI(+)-MS (*m*/*z*): 301.9 ($C_{82}H_{166}N_4$/4). FT-IR (KBr) ν_{max}: 3436, 3010, 2919, 2851, 1622, 1468, 1380, 1255, 1002, 722.