

Table S1. Interaction of 5-hydroxyethyl-4-methyl 1,3-thiazole (**1**) with haloalkanes under PTC conditions.

Haloalkane	Catalyst	Time h	Product	Yield %	Cr/Al ^a
C ₇ H ₁₅ Br	Aliquat ^R 336	14	2	63	1.1
C ₇ H ₁₅ Br	18-Crown-6	4	2	67	
C ₁₀ H ₂₁ I	Aliquat ^R 336	14	3	69	1.2
C ₁₀ H ₂₁ I	18-Crown-6	2	3	83	
C ₁₁ H ₂₃ I	Aliquat ^R 336	2	4	55	
C ₁₁ H ₂₃ I	Aliquat ^R 336	16	4	88	
C ₁₁ H ₂₃ Cl/Na	Aliquat ^R 336	43	4	2	
C ₁₈ H ₃₇ Br	Aliquat ^R 336	54	5	24	1.9
C ₁₈ H ₃₇ Br	18-Crown-6	45	5	45	

^a Ratio of product yields using different catalysts: 18-Crown-6 (Cr), AliquatR336 (Al).

Table S2. Synthesis of quaternary ammonium salts **7–13**.

Compound	R	R'	X	Time h	Yield %
7	C ₇ H ₁₅	CH ₃	I	4	51
8	C ₇ H ₁₅	C ₇ H ₁₅	Br	24	55
9	C ₇ H ₁₅	C ₁₀ H ₂₁	I	24	33
10	C ₁₀ H ₂₁	CH ₃	I	8	45
11	C ₁₀ H ₂₁	C ₇ H ₁₅	Br	24	18
12	C ₁₀ H ₂₁	C ₁₀ H ₂₁	I	24	69
13	C ₁₁ H ₂₃	CH ₃	I	7	12

Table S3. Tumour growth dynamics (mm³) during experiment (7–17 days).

Control/day	7	8	9	10	11	14	15	16	17
average	3461	6333	15671	16789	30139	40860	41747	38602	45931
stdev	813	3763	7508	11130	13648	23780	23180	19840	25729
Compound 13 /day	7	8	9	10	11	14	15	16	17
average	3759	6956	6884	10293	17239	18709	23901	23600	30058
stdev	1191	4450	3034	5045	9672	6862	4356	4592	5553
Inh%	-9	-10	56	39	43	54	43	39	35
ttest	0.650	0.811	0.035	0.240	0.101	0.073	0.120	0.127	0.197

Synthetic procedures, spectral and elemental analysis data of the synthesized compounds

5-(2-Heptyloxyethyl)-4-methyl-1,3-thiazole (2): From 5-(2-hydroxyethyl)-4-methyl-1,3-thiazole (**1**) (0.50 g, 3.5 mmol), 1-bromoheptane (0.66 g, 3.7 mmol), potassium hydroxide (0.98 g, 17.5 mmol) and Aliquat 336 (71 mg, 0.17 mmol) or of 18-Crown-6 (46 mg, 0.17 mmol) in dry benzene (3 ml). Product was isolated as light yellow oily substance. Yield: 0.53 g (63%) using Aliquat 336, 0.57 g (67%) using 18-Crown-6. ^1H NMR (400 MHz; CDCl_3) δ : 0.87 (3 H, t, $J = 6.8$ Hz, Me), 1.28 (10 H, br s, CH_2), 1.58 (2 H, m, CH_2), 2.39 (3 H, s, 4-Me), 3.00 (2 H, t, $J = 6.6$ Hz, $\alpha\text{-CH}_2$), 3.42 (2 H, t, $J = 6.6$ Hz, OCH_2), 3.58 (2 H, t, $J = 6.6$ Hz, $\beta\text{-CH}_2\text{O}$), 8.55 (1 H, s, 2-H). ^{13}C NMR (100 MHz, CDCl_3) δ : 14.0 (Me), 14.9 (4-Me), 22.6, 26.1 (CH_2), 27.0 ($\alpha\text{-CH}_2$), 29.1, 29.7, 31.8 (CH_2), 70.5 ($\beta\text{-C}$), 71.2 (O-C), 128.1, 149.1 (4,5-C), 149.6 (2-C). GC-MS, m/z : 241 (M^+ , 27%), 142 (5, $\text{M} - \text{C}_7\text{H}_{15}$), 126 (11, $\text{M} - \text{OC}_7\text{H}_{15}$), 113 (27, $\text{M} - \text{CH}_2\text{OC}_7\text{H}_{15} + 1$), 97 (22, $\text{M} - \text{CH}_2\text{OC}_7\text{H}_{15} - \text{CH}_3 - 1$), 57 (100). Found: C, 64.55; H, 9.58; N, 5.82; S, 13.32. Calc. for $\text{C}_{13}\text{H}_{23}\text{NOS}$: C, 64.68; H, 9.60; N, 5.80; S, 13.28%.

5-(2-Decyloxyethyl)-4-methyl-1,3-thiazole (3): From 5-(2-hydroxyethyl)-4-methyl-1,3-thiazole (**1**) (0.50 g, 3.5 mmol), 1-iododecane (0.98 g, 3.7 mmol), potassium hydroxide (0.98 g, 17.5 mmol) and Aliquat 336 (71 mg, 0.17 mmol) or 18-Crown-6 (46 mg, 0.17 mmol) in dry benzene (3 ml). Product was isolated as light yellow oily substance. Yield: 0.68 g (69%) using Aliquat 336, 0.83 g (83%) using 18-Crown-6. ^1H NMR (400 MHz, CDCl_3) δ : 0.87 (3 H, t, $J = 7.0$ Hz, Me), 1.26 (16 H, br s, CH_2), 1.56 (2 H, m, CH_2), 2.39 (3 H, s, 4-Me), 3.00 (2 H, t, $J = 6.6$ Hz, $\alpha\text{-CH}_2$), 3.42 (2 H, t, $J = 6.6$ Hz, OCH_2), 3.57 (2H, t, $J = 6.6$ Hz, $\beta\text{-CH}_2\text{O}$), 8.55 (1 H, s, 2-H). ^{13}C NMR (100 MHz, CDCl_3) δ : 14.1 (Me), 14.9 (4-Me), 22.7, 26.1 (CH_2), 27.0 ($\alpha\text{-CH}_2$), 29.3, 29.4, 29.5, 29.6, 29.7, 31.9 (CH_2), 70.6 ($\beta\text{-C}$), 71.2 (OCH_2), 128.1, 149.1 (4,5-C), 149.6 (2-C). GC-MS, m/z : 283 (M^+ , 30%), 142 (36, $\text{M} - \text{C}_{10}\text{H}_{21}$), 126 (22, $\text{M} - \text{OC}_{10}\text{H}_{21}$), 113 (44, $\text{M} - \text{CH}_2\text{OC}_{10}\text{H}_{21} + 1$), 99 (22, $\text{M} - \text{CH}_2\text{OC}_{10}\text{H}_{21} - \text{Me} + 1$), 85 (87), 57 (100). Found: C, 67.88; H, 10.34; N, 4.91; S, 11.28. Calc. for $\text{C}_{16}\text{H}_{29}\text{NOS}$: C, 67.79; H, 10.31; N, 4.94; S, 11.31%.

4-Methyl-5-(2-undecyloxyethyl)-1,3-thiazole (4): From 5-(2-hydroxyethyl)-4-methyl-1,3-thiazole (**1**) (0.25 g, 1.7 mmol), 1-haloundecane (1.8 mmol), potassium hydroxide (0.48 g, 8.5 mmol), and Aliquat 336 (34 mg, 0.085 mmol) in dry benzene (4 ml). Product was isolated as yellow oily substance. Yield: 0.28 g (55%) in case of using 1-iodoundecane under heating for 2 h, 0.45 g (88%) under heating for 16 h and 2% in case of using 1-chloroundecane under heating for 43 h. ^1H NMR (400 MHz, CDCl_3) δ : 0.85 (3H, t, $J = 7.0$ Hz, Me), 1.23 (18H, br s, CH_2), 1.54 (2H, m, CH_2), 2.36 (3H, s, 4-Me), 2.97 (2H, t, $J = 6.6$ Hz, $\alpha\text{-CH}_2$), 3.40 (2H, t, $J = 6.6$ Hz, OCH_2), 3.55 (2H, t, $J = 6.6$ Hz, $\beta\text{-CH}_2\text{O}$), 8.52 (1H, s, 2-H). ^{13}C NMR (100 MHz, CDCl_3) δ : 14.0 (Me), 14.9 (4-Me), 22.6, 26.1 (CH_2), 27.0 ($\alpha\text{-CH}_2$), 29.3, 29.4, 29.55, 29.63, 31.8 (CH_2), 70.5 ($\beta\text{-C}$), 71.2 (OCH_2), 128.0, 149.1 (4,5-C), 149.5 (2-C). GC-MS, m/z : 297 (M^+ , 37%), 142 (43, $\text{M} - \text{C}_{11}\text{H}_{23}$), 126 (27, $\text{M} - \text{OC}_{11}\text{H}_{23}$), 113 (44, $\text{M} - \text{CH}_2\text{OC}_{11}\text{H}_{23} + 1$), 99 (22, $\text{M} - \text{CH}_2\text{OC}_{11}\text{H}_{23} - \text{Me} + 1$), 57 (100). Found: C 68.55, H 10.53, N 4.72, S 10.75. Calc. for $\text{C}_{17}\text{H}_{31}\text{NOS}$: C 68.63, H 10.50, N 4.71, S 10.78%.

4-Methyl-5-(2-octadecyloxyethyl)-1,3-thiazole (5): From 5-(2-hydroxyethyl)-4-methyl-1,3-thiazole (**1**) (0.50 g, 3.5 mmol), 1-bromooctadecane (1.22 g, 3.7 mmol), potassium hydroxide (0.98 g, 17.5 mmol) and Aliquat 336 (71 mg, 0.17 mmol) or 18-Crown-6 (46 mg, 0.17 mmol) in dry benzene (3 ml). Product was isolated as white oily substance and gave white crystalline powder after crystallization from methanol, mp 39–41°C (MeOH). Yield: 0.33 g (24%) using

Aliquat 336, 0.65 g (45%) using 18-Crown-6. ^1H NMR (400 MHz, CDCl_3) δ : 0.87 (3H, t, J = 6.9 Hz, Me), 1.24 (30H, br s, CH_2), 1.56 (2H, m, CH_2), 2.39 (3H, s, 4-Me), 3.00 (2H, t, J = 6.6 Hz, $\alpha\text{-CH}_2$), 3.42 (2H, t, J = 6.6 Hz, OCH_2), 3.57 (t, J = 6.6 Hz, 2H, $\beta\text{-CH}_2\text{O}$), 8.55 (1H, s, 2-H). ^{13}C NMR (100 MHz, CDCl_3) δ : 14.1 (Me), 15.0 (4-Me), 22.7, 26.2 (CH_2), 27.1 ($\alpha\text{-CH}_2$), 29.4, 29.5, 29.6, 29.7, 31.9 (CH_2), 70.6 ($\beta\text{-C}$), 71.3 (OCH_2), 128.1, 149.2 (4,5-C), 149.6 (2-C). GC-MS, m/z : 395 (M^+ , 32%), 142 (56, $\text{M} - \text{C}_{18}\text{H}_{37}$), 113 (47, $\text{M} - \text{CH}_2\text{OC}_{18}\text{H}_{37}$), 85 (57), 57 (100). Found: C 72.94, H 11.43, N 3.53, S 8.12. Calc. for $\text{C}_{24}\text{H}_{45}\text{NOS}$: C 72.85, H 11.46, N 3.54, S 8.10%.

3,4-Dimethyl-5-(2-heptyloxyethyl)-1,3-thiazol-3-ium iodide (7)

(A): From 4-methyl-5-(2-heptyloxyethyl)-1,3-thiazole (**2**) (0.40 g, 1.7 mmol) and iodomethane (0.71 g, 5.0 mmol). Product was isolated as light yellow solid substance and gave white crystalline powder after crystallization from diethyl ether-methanol, mp 53–55°C (Et_2O –MeOH). Yield: 0.33 g (51%). ^1H NMR (400 MHz, CDCl_3) δ : 0.88 (3H, t, J = 7.0 Hz, Me), 1.30 (8H, br s, CH_2), 1.58 (2H, m, CH_2), 2.53 (3H, s, 4-Me), 3.08 (2H, t, J = 5.5 Hz, $\alpha\text{-CH}_2$), 3.46 (2H, t, J = 6.7 Hz, OCH_2), 3.65 (2H, t, J = 5.5 Hz, $\beta\text{-CH}_2\text{O}$), 4.41 (3H, s, N^+Me), 10.96 (1H, s, 2-H). ^{13}C NMR (100 MHz, CDCl_3) δ : 12.6 (4-Me), 14.0 (Me), 27.9 ($\alpha\text{-CH}_2$), 22.5, 26.0, 29.0, 29.5, 31.7 (CH_2), 41.6 (N^+Me), 68.1 ($\beta\text{-CH}_2\text{O}$), 71.6 (O-C), 135.1 (5-C), 141.9 (4-C), 157.0 (2-C). LC-MS, m/z : 257 (70%, $\text{M} - \text{I} + 1$), 256 (100, $\text{M} - \text{I}$). Found: C 43.80, H 6.82, N 3.65, S 8.38. Calc. for $\text{C}_{14}\text{H}_{26}\text{INOS}$: C 43.87, H 6.84, N 3.64, S 8.36%.

3-Heptyl-5-(2-heptyloxyethyl)-4-methyl-1,3-thiazol-3-ium bromide (8)

(B): From 4-methyl-5-(2-heptyloxyethyl)-1,3-thiazole (**2**) (0.20 g, 0.83 mmol) and 1-bromoheptane (0.15 g, 0.83 mmol) under heating in acetonitrile for 24 h. Product was isolated as light yellow oily substance. Yield: 0.21 g (55%). ^1H NMR (400 MHz, CDCl_3) δ : 0.87 (6H, m, Me), 1.27 (16H, br s, CH_2), 1.56 (2H, m, $\text{CH}_2\text{-C-O}$), 1.92 (2H, m, $\text{CH}_2\text{-C-N}^+$), 2.48 (3H, s, 4-Me), 3.07 (2H, t, J = 5.5 Hz, $\alpha\text{-CH}_2$), 3.46 (2H, t, J = 6.7 Hz, OCH_2), 3.65 (2H, t, J = 5.5 Hz, $\beta\text{-CH}_2\text{O}$), 4.74 (2H, t, J = 7.6 Hz, CH_2N^+), 11.37 (1H, s, 2-H). ^{13}C NMR (100 MHz, CDCl_3) δ : 11.8 (4-Me), 14.0, 14.9 (Me), 29.5 ($\alpha\text{-CH}_2$), 22.5, 27.8, 28.1, 28.4, 28.7, 30.4, 31.5, 31.7, 32.8, 45.1 (CH_2), 53.6 (CH_2N^+), 68.2 ($\beta\text{-CH}_2\text{O}$), 71.7 (O- CH_2), 135.4 (5-C), 140.5 (4-C), 158.6 (2-C). LC-MS, m/z : 340 (100%, $\text{M} - \text{Br}$). Found: C 57.25, H 9.07, N 3.34, S 7.64. Calc. for $\text{C}_{20}\text{H}_{38}\text{BrNOS}$: C 57.13, H 9.10, N 3.33, S 7.62%.

3-Decyl-5-(2-heptyloxyethyl)-4-methyl-1,3-thiazol-3-ium iodide (9)

(B): From 4-methyl-5-(2-heptyloxyethyl)-1,3-thiazole (**2**) (0.20 g, 0.83 mmol) and 1-iododecane (0.22 g, 0.83 mmol) under heating in acetonitrile for 24 h. Product was isolated as yellow oily substance. Yield: 0.14 g (33%). ^1H NMR (400 MHz, CDCl_3) δ : 0.87 (6H, m, Me), 1.26 (22H, br s, CH_2), 1.57 (2H, m, $\text{CH}_2\text{-C-O}$), 1.74 (2H, m, $\text{CH}_2\text{-C-N}^+$), 2.50 (3H, s, 4-Me), 3.08 (2H, t, J = 5.6 Hz, $\alpha\text{-CH}_2$), 3.46 (2H, t, J = 6.6 Hz, OCH_2), 3.66 (2H, t, J = 5.6 Hz, $\beta\text{-CH}_2\text{O}$), 4.71 (2H, t, J = 7.7 Hz, CH_2N^+), 11.03 (1H, s, 2-H). ^{13}C NMR (100 MHz, CDCl_3) δ : 12.2 (4-Me), 14.9 (Me), 29.6 ($\alpha\text{-CH}_2$), 26.2, 26.9, 27.9, 28.9, 29.0, 29.3, 29.4, 30.3, 31.7, 31.8, 32.6, 35.6, 45.2 (CH_2), 53.8 (CH_2N^+), 68.2 ($\beta\text{-CH}_2\text{O}$), 71.2 (O- CH_2), 135.7 (5-C), 140.8 (4-C), 157.5 (2-C). LC-MS, m/z : 383 (70%, $\text{M} - \text{I} + 1$), 382 (100, $\text{M} - \text{I}$). Found: C 54.28, H 8.71, N 2.75, S 6.27. Calc. for $\text{C}_{23}\text{H}_{44}\text{INOS}$: C 54.21, H 8.70, N 2.75, S 6.29%.

5-(2-Decyloxyethyl)-3,4-dimethyl-1,3-thiazol-3-ium iodide (10)

(A): From 4-methyl-5-(2-decyloxyethyl)-1,3-thiazole (**3**) (0.47 g, 1.7 mmol) and iodomethane (0.57 g, 4.0 mmol). Product was isolated as white solid substance and gave white crystalline powder after crystallization from diethyl ether, mp 90–92°C (Et_2O). Yield: 0.27 g (45%). ^1H NMR (400 MHz, CDCl_3) δ : 0.87 3H, (t, J = 6.9 Hz, Me), 1.26 (14H, br s, CH_2), 1.57 (2H, m, CH_2), 2.52

(3H, s, 4-Me), 3.07 (2H, t, J = 5.5 Hz, α -CH₂), 3.46 (2H, t, J = 6.6 Hz, OCH₂), 3.64 (2H, t, J = 5.5 Hz, β -CH₂O), 4.40 (3H, s, N⁺CH₃), 10.98 (1H, s, 2-H). ¹³C NMR (100 MHz, CDCl₃) δ : 12.6 (4-Me), 14.0 (Me), 27.9 (α -CH₂), 22.6, 26.1, 29.3, 29.4, 29.5, 31.9 (CH₂), 41.6 (N⁺CH₃), 65.2 (β -CH₂O), 68.2 (O-C), 135.2 (5-C), 141.8 (4-C), 157.2 (2-C). LC-MS, m/z : 299 (100%, M – I + 1), 298 (50, M – I). Found: C 47.89, H 7.57, N 3.28, S 7.56. Calc. for C₁₇H₃₂INOS: C 48.00, H 7.58, N 3.29, S 7.54%

5-(2-Decyloxyethyl)-3-heptyl-4-methyl-1,3-thiazol-3-ium bromide (11)

(B): From 4-methyl-5-(2-decyloxyethyl)-1,3-thiazole (**3**) (0.20 g, 0.71 mmol) and 1-bromoheptane (0.32 g, 0.71 mmol) under heating in acetonitrile for 24 h. Product was isolated as light yellow oily substance. Yield: 0.06 g (18%). ¹H NMR (400 MHz, CDCl₃) δ : 0.87 (6H, m, Me), 1.26 (22H, br s, CH₂), 1.56 (2H, m, CH₂-C-O), 1.93 (2H, m, CH₂-C-N⁺), 2.48 (3H, s, 4-Me), 3.07 (2H, t, J = 5.5 Hz, α -CH₂), 3.46 (2H, t, J = 6.7 Hz, OCH₂), 3.64 (t, J = 5.5 Hz, 2H, β -CH₂O), 4.76 (2H, t, J = 7.6 Hz, CH₂N⁺), 11.50 (1H, s, 2-H). ¹³C NMR (100 MHz, CDCl₃) δ : 11.9 (4-Me), 14.8 (Me), 29.7 (α -CH₂), 22.5, 27.0, 27.8, 28.7, 29.4, 30.4, 31.5, 45.2 (CH₂), 53.6 (CH₂N⁺), 68.2 (β -CH₂O), 71.7 (O-CH₂), 135.4 (5-C), 140.4 (4-C), 157.5 (2-C). LC-MS, m/z : 382 (100%, M – Br). Found: C 59.65, H 9.56, N 3.04, S 6.91. Calc. for C₂₃H₄₄BrNOS: C 59.72, H 9.59, N 3.03, S 6.93%.

3-Decyl-5-(2-decyloxyethyl)-4-methyl-1,3-thiazol-3-ium iodide (12)

(B): From 4-methyl-5-(2-decyloxyethyl)-1,3-thiazole (**3**) (0.20 g, 0.71 mmol) and 1-iododecane (0.18 g, 0.71 mmol) under heating in acetonitrile for 24 h. Product was isolated as yellow oily substance. Yield 0.27 g (69%). ¹H NMR (400 MHz, CDCl₃) δ : 0.87 (6H, m, Me), 1.26 (28H, br s, CH₂), 1.57 (2H, m, CH₂-C-O), 1.74 (2H, m, CH₂-C-N⁺), 2.49 (3H, s, 4-Me), 3.07 (2H, t, J = 5.6 Hz, α -CH₂), 3.46 (2H, t, J = 6.7 Hz, OCH₂), 3.66 (2H, t, J = 5.6 Hz, β -CH₂O), 4.70 (2H, t, J = 7.6 Hz, CH₂N⁺), 11.03 (1H, s, 2-H). ¹³C NMR (100 MHz, CDCl₃) δ : 12.1 (4-Me), 14.9 (Me), 29.7 (α -CH₂), 26.2, 26.9, 27.9, 28.9, 29.0, 29.3, 29.4, 30.3, 32.6, 45.2 (CH₂), 53.8 (CH₂N⁺), 68.1 (β -CH₂O), 71.8 (O-CH₂), 135.7 (5-C), 140.8 (4-C), 157.5 (2-C). LC-MS, m/z : 425 (90%, M – I + 1), 424 (100, M – I). Found: C 56.51, H 9.16, N 2.54, S 5.79. Calc. for C₂₆H₅₀INOS: C 56.60, H 9.14, N 2.54, S 5.81%.

3,4-Dimethyl-5-(2-undecyloxyethyl)-1,3-thiazol-3-ium iodide (13)

(B): From 5-(2-decyloxyethyl)-4-methyl-1,3-thiazole (**4**) (0.35 g, 1.2 mmol) and iodomethane (1.02 g, 7.2 mmol) under heating in ether for 8 h. Product was isolated as white solid substance and gave white crystalline powder after crystallization from diethyl ether, mp: 90–92°C (Et₂O). Yield: 0.06 g (12%). ¹H NMR (400 MHz, CDCl₃) δ : 0.87 (3H, t, J = 6.9 Hz, CH₃), 1.26 (16H, br s, CH₂), 1.56 (2H, m, CH₂), 2.52 (3H, s, 4-CH₃), 3.07 (2H, t, J = 5.5 Hz, α -CH₂), 3.45 (2H, t, J = 6.6 Hz, OCH₂), 3.64 (2H, t, J = 5.5 Hz, β -CH₂O), 4.39 (3H, s, N⁺CH₃), 10.98 (1H, s, 2-H). ¹³C NMR (100 MHz, CDCl₃) δ : 12.6 (4-Me), 14.1 (Me), 27.9 (α -CH₂), 22.7, 26.1, 29.3, 29.4, 29.5, 29.55, 29.58, 31.9 (CH₂), 41.6 (N⁺CH₃), 65.2 (β -CH₂O), 68.2 (O-C), 135.2 (5-C), 141.8 (4-C), 157.2 (2-C). LC-MS, m/z : 313 (100%, M – I + 1), 312 (40, M – I). Found: C 49.25, H 7.79, N 3.20, S 7.32. Calc. for C₁₈H₃₄INOS: C 49.20, H 7.80, N 3.19, S 7.30%.