Supporting Information

A New Class of Selective Myocardial Calcium Channel Modulators. 2. The Role of the Acetal Chain in Oxadiazol-3-one Derivatives

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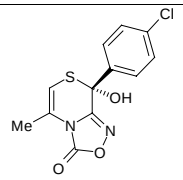
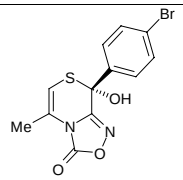
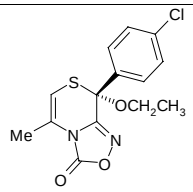
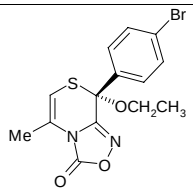
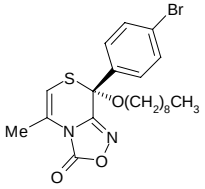
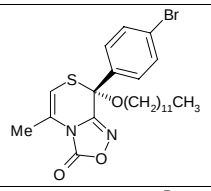
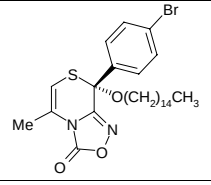
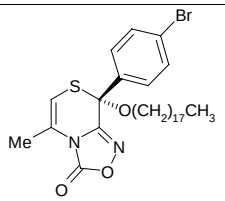
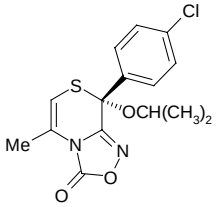
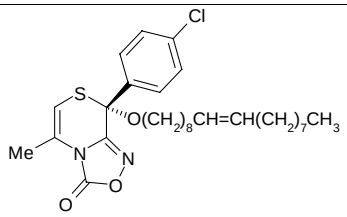
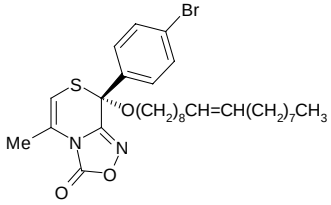
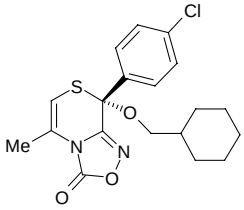
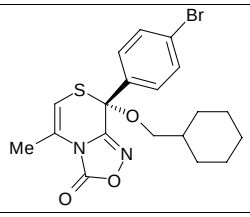
Table S1. Calculated pK_a values for compounds from Training Set and Test Set.

Compounds from the Training Set	Calculated pK_a	Compounds from the Test Set	Calculated pK_a
8c	8.53	**Diltiazem (t01)**	8.38
11d	9.37	**10d (t11)**	9.02
24b	8.52	**11g (t12)**	9.37
		13 (t13)	8.49
		24a (t15)	8.52

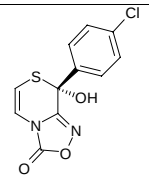
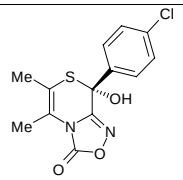
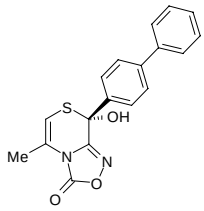
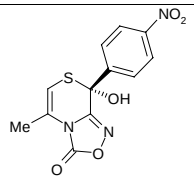
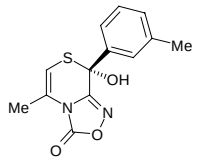
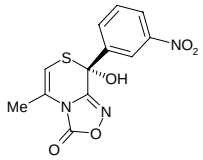
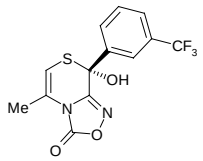
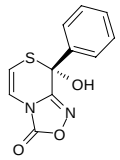
Table S2. Data used as Training Set extracted from the present paper.

Compound	Structure	EC_{50} (μM)	pEC_{50} [a]
1a [b]		0.80	0.097
1b [c]		0.32	0.495
5a		0.27	0.569
5b		0.04	1.398
10b		0.35	0.456
11b		0.13	0.886
12b		0.42	0.377

Compound	Structure	EC_{50} (μM)	pEC_{50} [a]
13b		0.97	0.013
14a		0.22	0.658
18a	 (Z-isomer)	0.87	0.060
18b	 (Z-isomer)	1.26	-0.100
20a		0.24	0.620
20b		0.19	0.721

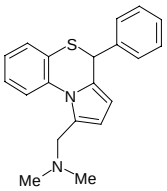
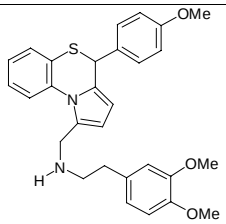
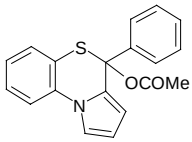
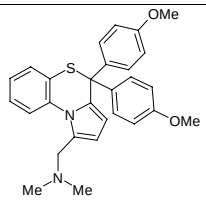
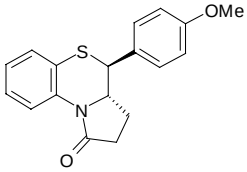
[a] Negative Inotropic Potency pEC_{50} calculated as –log EC_{50}, where EC_{50} (μM) values of negative inotropic potency were computed from log concentration-response curves (Probit analysis according to Litchfield and Wilcoxon with n = 6-8) as reported in Table 1. [b] **1a** is reported in this paper but it is taken from reference 3, named as **4a**. [c] **1b** is reported in this paper but it is taken from reference 3, named as **4f**.

Table S3. Data used as Training Set extracted from reference 3.

Compound	Structure	EC_{50} (μM)	pEC_{50} [a]
4B		4.07	-0.610
4C		1.42	-0.152
4I		2.65	-0.423
4L		1.65	-0.217
4N		0.72	0.143
4P		1.76	-0.246
4Q		2.17	-0.336
6		6.58	-0.818

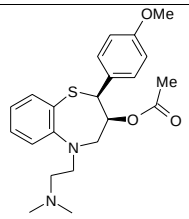
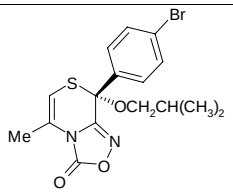
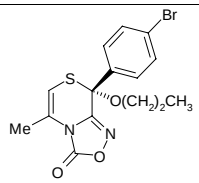
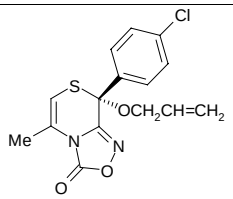
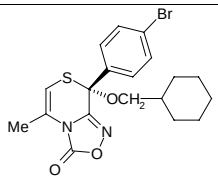
[a] Negative Inotropic Potency pEC_{50} calculated as –log EC_{50}, where EC_{50} (μM) values of negative inotropic potency were computed from log concentration-response curves (Probit analysis according to Litchfield and Wilcoxon with n = 6-8) as reported in reference 3.

Table S4. Tabular data used as Training Set extracted from reference 11.

Compound	Structure	EC_{50} (μM)	pEC_{50} [a]
8c		1.5	-0.176
11d		0.45	0.347
22a		0.38	0.420
24b		0.73	0.137
28b		1.2	-0.079

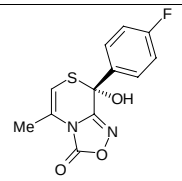
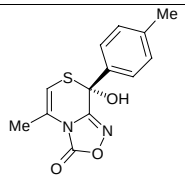
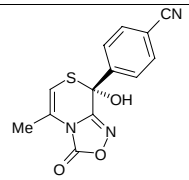
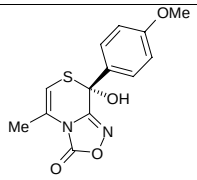
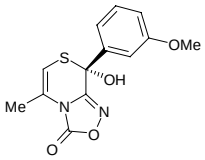
[a] Negative Inotropic Potency pEC_{50} calculated as –log EC_{50}, where EC_{50} (μM) values of negative inotropic potency were computed from log concentration-response curves (Probit analysis according to Litchfield and Wilcoxon with n = 5-7) as reported in reference 11.

Table S5. Data used as Test Set extracted from the present paper.

Compound	Original Name	Structure	EC_{50} (µM)	pEC_{50} [a]
t01	Diltiazem		0.79	0.102
t02	4b		0.31	0.509
t03	6b		0.41	0.387
t04	15a		0.37	0.432
t05	19b		0.59	0.229

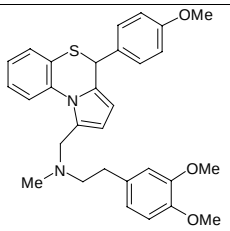
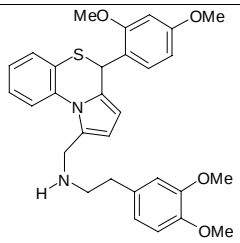
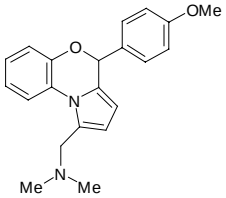
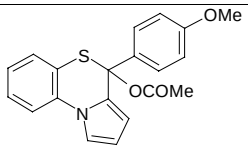
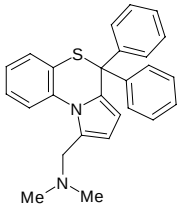
[a] Negative Inotropic Potency pEC_{50} calculated as –log EC_{50}, where EC_{50} (µM) values of negative inotropic potency were computed from log concentration-response curves (Probit analysis according to Litchfield and Wilcoxon with n = 6-8) as reported in Table 1.

Table S6. Data used as Test Set extracted from reference 3.

Compound	Original Name	Structure	EC_{50} (μM)	pEC_{50} [a]
t06	4g		1.21	-0.083
t07	4h		0.57	0.244
t08	4j		0.76	0.119
t09	4k		0.52	0.284
t10	4o		0.49	0.310

[a] Negative Inotropic Potency pEC_{50} calculated as –log EC_{50}, where EC_{50} (μM) values of negative inotropic potency were computed from log concentration-response curves (Probit analysis according to Litchfield and Wilcoxon with n = 6-8) as reported in reference 3.

Table S7. Data used as Test Set extracted from reference 11.

Compound	Original Name	Structure	EC_{50} (μM)	pEC_{50} [a]
t11	10d		0.84	0.076
t12	11g		0.56	0.252
t13	13		0.92	0.036
t14	22b		0.24	0.620
t15	24a		0.89	0.051

[a] Negative Inotropic Potency pEC_{50} calculated as –log EC_{50}, where EC_{50} (μM) values of negative inotropic potency were computed from log concentration-response curves (Probit analysis according to Litchfield and Wilcoxon with n = 5-7) as reference 11.

Table S8. ^{1}H NMR, ^{13}C NMR, ESI-MS and EI-MS data for compounds **5a**-**20a**, **4b**-**20b**.

8-(4-Bromophenyl)-8-isobutoxy-5-methy-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (4b). ^{1}H NMR: δ 0.85 (6H, d, *J* = 6.8 Hz, 2xCH_3), 1.83 (1H, m, CH), 2.40 (3H, d, *J* = 1.5 Hz, 5-CH_3), 3.11 (1H, m, OCH_2), 3.33 (1H, m, OCH_2), 6.22 (1H, q, *J* = 1.5 Hz, H-6), 7.52 (2H, m, part AA' of the AA'XX' system, H-Ar), 7.71 (2H, m, part XX' of the AA'XX' system, H-Ar). ^{13}C NMR: δ 16.1 (q, 5-CH_3), 18.7 (q, 2xCH_3), 27.5 (d, CH), 70.4 (t, OCH_2), 82.0 (s, C-8), 103.4 (d, C-6), 123.1 (s, C-4'), 129.4 (d, C-2', C-6'), 129.6 (s, C-5), 131.5 (d, C-3', C-5'), 132.6 (s, C-1'), 154.1 (s, C-8a), 154.4 (s, C-3). EI: *m/z* (%) 398-396 (M^+, 13), 185-183 (75), 157 (55), 155 (33), 113 (20), 104 (13), 76 (29), 75 (13), 57 (100). ESI: *m/z* 419.3 (M + Na^+).

8-(4-Chlorophenyl)-8-ethoxy-5-methyl-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (5a). ^{1}H NMR: δ 1.17 (3H, t, *J* = 7.0 Hz, CH_3), 2.41 (3H, d, *J* = 1.1 Hz, 5-CH_3), 3.40 (1H, m, OCH_2), 3.57 (m, 1H, OCH_2), 6.22 (1H, q, *J* = 1.1 Hz, H-6), 7.59 (4H, m, H-Ar). ^{13}C NMR: δ 14.6 (q, CH_3), 16.5 (q, 5-CH_3), 60.8 (t, OCH_2), 82.0 (s, C-8), 103.3 (d, C-6), 128.8 (d, C-3', C5'), 129.3 (d, C-2', C-6'), 129.6 (s, C-5), 132.5 (s, C-1'), 134.6 (s, C-4'), 154.2 (s, C-8a), 154.6 (s, C-3). EI: m/z (%) 326-324 (M^+, 22), 279 (17), 235 (12), 141 (33), 139 (100), 113 (18), 111 (29), 75 (19), 45 (16). ESI: *m/z* 347.3 (M + Na^+).

8-(4-Bromophenyl)-8-ethoxy-5-methyl-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (5b). ^{1}H NMR: δ 1.16 (3H, t, *J* = 7.0 Hz, CH_3), 2.40 (3H, d, *J* = 1.1 Hz, 5-CH_3), 3.39 (1H, m, OCH_2), 3.57 (1H, m, OCH_2), 6.22 (1H, q, *J* = 1.1 Hz, H-6), 7.52 (2H, m, part AA' of the AA'XX' system, H-Ar), 7.71 (2H, m, part XX' of the AA'XX' system, H-Ar). ^{13}C NMR: δ 14.6 (q, CH_3), 16.5 (q, 5-CH_3), 60.8 (t, OCH_2), 82.1 (s, C-8), 103.2 (d, C-6), 123.2 (s, C-4'), 129.4 (d, C-2', C-6'), 129.4 (s, C-5), 131.6 (d, C-3', C-5'), 132.8 (s, C-1'), 154.0 (s, C-8a), 154.4 (s, C-3). ESI: *m/z* 391.3 (M + Na^+).

8-(4-Chlorophenyl)-5-methyl-8-propoxy-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (6a). ^{1}H NMR: δ 0.84 (3H, t, *J* = 7.3 Hz, CH_3), 1.56 (2H, m, CH_2), 2.40 (3H, d, *J* = 1.3 Hz, 5-CH_3), 3.29 (1H, m, OCH_2), 3.49 (1H, m, OCH_2), 6.22 (1H, q, *J* = 1.3 Hz, H-6), 7.58 (4H, m, H-Ar). ^{13}C NMR: δ 10.3 (q, CH_3), 16.4 (q, 5-CH_3), 22.0 (t, CH_2), 66.2 (t, OCH_2), 82.0 (s, C-8), 103.3 (d, C-6), 128.7 (d, C-3', C-5'), 129.2 (d, C-2', C-6'), 129.6 (s, C-5), 132.2 (s, C-1'), 134.5 (s, C-4'), 154.2 (s, C-8a), 154.5 (s, C-3). EI: m/z (%) 340-338 (M^+, 15), 279 (14), 157 (19), 141 (34), 139 (100), 113 (25), 111 (54), 75 (18), 45 (20), 43 (61), 41 (37), 39 (16). ESI: *m/z* 361.3 (M + Na^+).

8-(4-Bromophenyl)-5-methyl-8-propoxy-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (6b). ^{1}H NMR: δ 0.85 (3H, t, *J* = 7.2 Hz, CH_3), 1.56 (2H, m, CH_2), 2.40 (3H, d, *J* = 1.2 Hz, 5-CH_3), 3.30 (1H, m, OCH_2), 3.49 (1H, m, OCH_2), 6.22 (1H, q, *J* = 1.2 Hz, H-6), 7.53 (2H, m, part AA' of the AA'XX' system, H-Ar), 7.71 (2H, m, part XX' of the AA'XX' system, H-Ar). ^{13}C NMR: δ 10.2 (q, CH_3), 16.4 (q, 5-CH_3), 22.0 (t, CH_2,), 66.2 (t, OCH_2), 82.0 (s, C-8,), 103.4 (d, C-6), 123.3 (s, C-4'), 129.6 (d, C-2', C-6'), 129.7 (s, C-5), 131.7 (d, C-3', C-5'), 132.8 (s, C-1'), 154.2 (s, C-8a), 154.6 (s, C-3). EI: m/z (%) 384-382 (M^+, 20), 323 (10), 185 (92), 183 (100), 157 (24), 155 (39), 113 (13), 76 (20), 75 (15), 50 (11), 45 (22), 43 (70), 41 (42), 39 (17). ESI: *m/z* 405.3 (M + Na^+).

8-Butoxy-8-(4-chlorophenyl)-5-methyl-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (7a). ^{1}H NMR: δ 0.85 (3H, t, *J* = 7.3 Hz, CH_3), 1.30 (2H, m, CH_2), 1.53 (2H, m, CH_2), 2.40 (3H, d, *J* = 1.2 Hz, 5-CH_3), 3.33 (1H, m, OCH_2), 3.54 (1H, m, OCH_2), 6.22 (1H, q, *J* = 1.2 Hz, H-6), 7.58 (4H, m, H-Ar). ^{13}C NMR: δ 13.4 (q, CH_3), 16.4 (q, 5-CH_3), 18.5 (t, CH_2), 30.6 (t, CH_2), 64.3 (t, OCH_2), 82.0 (s, C-8), 103.4 (d, C-6), 128.8 (d, C-3', C-5'), 129.3 (d, C-2', C-6'), 129.6 (s, C-5), 132.3 (s, C-1'), 134.6 (s, C-4'), 154.3 (s, C-8a), 154.6 (s, C-3). ESI: *m/z* 375.3 (M + Na^+).

8-(4-Bromophenyl)-8-butoxy-5-methyl-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (7b). ^{1}H NMR: δ 0.85 (3H, t, *J* = 7.3 Hz, CH_3), 1.29 (2H, m, CH_2), 1.51 (2H, m, CH_2), 2.40 (3H, d, *J* = 1.2 Hz, 5-CH_3), 3.33 (1H, m, OCH_2), 3.53 (1H, m, OCH_2), 6.23 (1H, q, *J* = 1.2 Hz, H-6), 7.52 (2H, m, part AA' of the AA'XX' system, H-Ar), 7.71 (2H, m, part XX' of the AA'XX' system, H-Ar). ^{13}C NMR: δ 13.5 (q, CH_3), 16.4 (q, 5-CH_3), 18.5 (t, CH_2), 30.6 (t, CH_2), 64.3 (t, OCH_3), 82.1 (s, C-8), 103.4 (d, C-6), 123.3 (s, C-4'), 129.6 (d, C-2', C-6'), 129.6 (s, C-5), 131.7 (d, C-3', C-5'), 132.7 (s, C-1'), 154.2 (s, C-8a),

154.6 (s, C-3). EI: m/z (%) 398-396 (M^+, 18), 323 (13), 185 (31), 184 (11), 183 (100), 157 (33), 113 (11), 76 (29), 75 (18), 71 (12), 50 (12), 45 (21), 41 (42), 39 (23). ESI: *m/z* 419.3 (M + Na^+).

8-(4-Chlorophenyl)-5-methyl-8-pentoxy-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (8a). ^{1}H NMR: δ 0.85 (3H, t, *J* = 7.1 Hz, CH_3), 1.22-1.27 (4H, m, 2xCH_2), 1.52-1.56 (2H, m, CH_2), 2.40 (3H, d, *J* = 1.4 Hz, 5-CH_3), 3.32 (1H, m, OCH_2), 3.53 (1H, m, OCH_2), 6.22 (1H, q, *J* = 1.4 Hz, H-6), 7.58 (4H, m, H-Ar). ^{13}C NMR: δ 13.8 (q, CH_3), 16.4 (q, 5-CH_3), 21.7 (t, CH_2), 27.5 (t, CH_2), 28.2 (t, CH_2), 64.5 (t, OCH_2), 82.0 (s, C-8), 103.4 (d, C-6), 128.8 (d, C-3', C-5'), 129.3 (d, C-2', C-6'), 129.6 (s, C-5), 132.3 (s, C-1'), 134.6 (s, C-4'), 154.3 (s, C-8a), 154.6 (s, C-3). ESI: *m/z* 389.3 (M + Na^+).

8-(4-Bromophenyl)-5-methyl-8-pentoxy-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (8b). ^{1}H NMR: δ 0.85 (3H, t, *J* = 6.8 Hz, CH_3), 1.22-1.27 (4H, m, 2xCH_2), 1.52-1.56 (2H, m, CH_2), 2.40 (3H, d, *J* = 1.2 Hz, 5-CH_3), 3.32 (1H, m, OCH_2), 3.53 (1H, m, OCH_2), 6.22 (1H, q, *J* = 1.2 Hz, H-6), 7.52 (2H, m, part AA' of the AA'XX' system, H-Ar), 7.71 (2H, m, part XX' of the AA'XX' system, H-Ar). ^{13}C NMR: δ 13.8 (q, CH_3), 16.4 (q, 5-CH_3), 21.7 (t, CH_2), 27.4 (t, CH_2), 28.2 (t, CH_2), 64.6 (t, OCH_2), 82.1 (s, C-8), 103.4 (d, C-6), 123.3 (s, C-4'), 129.6 (d, C-2', C-6'), 129.6 (s, C-5), 131.7 (d, C-3', C-5'), 132.7 (s, C-1'), 154.2 (s, C-8a), 154.6 (s, C-3). ESI: *m/z* 433.4 (M + Na^+).

8-(4-Chlorophenyl)-8-(hexyloxy)-5-methyl-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (9a). ^{1}H NMR: δ 0.85 (3H, t, *J* = 6.8 Hz, CH_3), 1.12-1.32 (6H, m, 3xCH_2), 1.49-1.60 (2H, m, CH_2), 2.40 (3H, d, *J* = 1.2 Hz, 5-CH_3), 3.32 (1H, m, OCH_2), 3.53 (1H, m, OCH_2), 6.22 (1H, q, *J* = 1.2 Hz, H-6), 7.58 (4H, m, H-Ar). ^{13}C NMR: δ 13.6 (q, CH_3), 16.2 (q, 5-CH_3), 21.8 (t, CH_2), 24.8 (t, CH_2), 28.4 (t, CH_2), 30.6 (t, CH_2), 64.5 (t, OCH_2), 82.0 (s, C-8), 103.4 (d, C-6), 128.6 (d, C-3', C-5'), 129.1 (d, C-2', C-6'), 129.5 (s, C-5), 132.2 (s, C-1'), 134.5 (s, C-4'), 154.2 (s, C-8a), 154.4 (s, C-3). EI: m/z (%) 380-382 (M^+, 13), 279 (10), 157 (29), 141 (27), 139 (87), 113 (15), 111 (32), 75 (11), 43 (100), 42 (10), 41 (43), 39 (13). ESI: *m/z* 403.4 (M + Na^+).

8-(4-Bromophenyl)-8-(hexyloxy)-5-methyl-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (9b). ^{1}H NMR: δ 0.85 (3H, m, *J* = 6.8 Hz, CH_3), 1.16-1.31 (6H, m, 3xCH_2), 1.48-1.60 (2H, m, CH_2), 2.40 (3H, d, *J* = 1.2 Hz, 5-CH_3), 3.32 (1H, m, OCH_2), 3.53 (1H, m, OCH_2), 6.22 (1H, q, *J* = 1.2 Hz, H-6), 7.52 (2H, m, part AA' of the AA'XX' system, H-Ar), 7.71 (2H, m, part XX' of the AA'XX' system, H-Ar). ^{13}C NMR: δ 13.5 (q, CH_3), 16.1 (q, 5-CH_3), 21.7 (t, CH_2), 24.7 (t, CH_2), 28.4 (t, CH_2), 30.6 (t, CH_2), 64.5 (t, OCH_2), 82.0 (s, C-8), 103.3 (d, C-6), 123.1 (s, C-4'), 129.4 (d, C-2', C-6'), 129.4 (s, C-5), 131.5 (d, C-3', C-5'), 132.7 (s, C-1'), 154.1 (s, C-8a), 154.4 (s, C-3). EI: m/z (%) 426-424 (M^+, 13), 185-183 (59), 157 (30), 155 (15), 76 (11), 57 (11), 55 (13), 43 (100), 41 (42), 39 (13). ESI: *m/z* 447.4 (M + Na^+).

8-(4-Chlorophenyl)-5-methyl-8-(nonyloxy)-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (10a). ^{1}H NMR: δ 0.85 (3H, t, *J* = 6.5 Hz, CH_3), 1.23 (12H, m, 6xCH_2), 1.47-1.59 (2H, m, CH_2), 2.40 (3H, t, *J* = 1.0 Hz, 5-CH_3), 3.32 (1H, m, OCH_2), 3.53 (1H, m, OCH_2), 6.21 (1H, q, *J* = 1.0 Hz, H-6), 7.58 (4H, m, H-Ar). ^{13}C NMR: δ 13.8 (q, CH_3), 16.4 (q, 5-CH_3), 22.0 (t, CH_2), 25.3 (t, CH_2), 28.5 (t, CH_2), 28.6 (t, 2xCH_2), 28.8 (t, CH_2), 31.2 (t, CH_2), 64.5 (t, OCH_2), 82.0 (s, C-8), 103.4 (d, C-6), 128.7 (d, C-3', C-5'), 129.3 (d, C-2', C-6'), 129.6 (s, C-5), 132.3 (s, C-1'), 134.6 (s, C-4'), 154.2 (s, C-8a), 154.6 (s, C-3). ESI: *m/z* 445.5 (M + Na^+).

8-(4-Bromophenyl)-5-methyl-8-(nonyloxy)-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (10b). ^{1}H NMR: δ 0.87 (3H, t, *J* = 6.8 Hz, CH_3), 1.24 (12H, m, 6xCH_2), 1.49-1.62 (2H, m, CH_2), 2.41 (3H, d, *J* = 1.2 Hz, 5-CH_3), 3.34 (1H, m, OCH_2), 3.54 (1H, m, OCH_2), 6.23 (1H, q, *J* = 1.2 Hz, H-6), 7.54 (2H, m, part AA' of the AA'XX' system, H-Ar), 7.72 (2H, m, part XX' of the AA'XX' system, H-Ar). ^{13}C NMR: δ 13.9 (q, CH_3), 16.4 (q, 5-CH_3), 22.0 (t, CH_2), 25.3 (t, CH_2), 28.5 (t, CH_2), 28.6 (t, 2xCH_2), 28.9 (t, CH_2), 31.2 (t, CH_2), 64.6 (t, OCH_2), 82.1 (s, C-8), 103.4 (d, C-6), 123.3 (s, C-4'), 129.6 (d, C-2', C-6'), 129.6 (s, C-5), 131.7 (d, C-3', C-5'), 132.7 (s, C-1'), 154.2 (s, C-8a), 154.6 (s, C-3). ESI: *m/z* 489.5 (M + Na^+).

8-(4-Chlorophenyl)-8-(dodecyloxy)-5-methyl-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (11a). ^{1}H NMR: δ 0.84 (3H, t, *J* = 6.8 Hz, CH_3), 1.22 (18H, m, 9xCH_2), 1.46-1.60 (2H, m, CH_2), 2.39 (3H, d, *J* = 1.0 Hz, 5-CH_3), 3.31 (1H, m, OCH_2), 3.50 (1H, m, OCH_2), 6.21 (1H, q, *J* = 1.0 Hz, H-6), 7.57 (4H, m,

H-Ar). ^{13}C NMR: δ 13.9 (q, CH_3), 16.4 (q, 5-CH_3), 22.0 (t, CH_2), 25.3 (t, CH_2), 28.5 (t, CH_2), 28.6 (t, 2xCH_2), 28.9 (t, 2xCH_2), 29.0 (t, 2xCH_2), 31.2 (t, CH_2), 64.5 (t, OCH_2), 82.0 (s, C-8), 103.4 (d, C-6), 128.8 (d, C-3', C-5'), 129.3 (d, C-2', C-6'), 129.6 (s, C-5), 132.3 (s, C-1'), 134.6 (s, C-4'), 154.3 (s, C-8a), 154.6 (s, C-3). EI: m/z (%) 466-464 (M^+, 7), 141 (11), 139 (100), 111 (12), 71 (17), 43 (45), 41 (33). ESI: *m/z* 487.6 (M + Na^+).

8-(4-Bromophenyl)-8-(dodecyloxy)-5-methyl-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (11b). ^{1}H NMR: δ 0.84 (3H, t, *J* = 6.8 Hz, CH_3), 1.22 (18H, m, 9xCH_2), 1.46-1.58 (2H, m, CH_2), 2.39 (3H, d, *J* = 1.2 Hz, 5-CH_3), 3.31 (1H, m, OCH_2), 3.52 (1H, m, OCH_2), 6.21 (1H, q, *J* = 1.2 Hz, H-6), 7.52 (2H, m, part AA' of the AA'XX' system, H-Ar), 7.70 (2H, m, part XX' of the AA'XX' system, H-Ar). ^{13}C NMR: δ 13.8 (q, CH_3), 16.4 (q, 5-CH_3), 22.0 (t, CH_2), 25.3 (t, CH_2), 28.5 (t, CH_2), 28.6 (t, 2xCH_2), 28.9 (t, 3xCH_2), 29.0 (t, CH_2), 31.2 (t, CH_2), 64.5 (t, OCH_2), 82.1 (d, C-8), 103.4 (d, C-6), 123.3 (s, C-4'), 129.5 (d, C-2', C-6'), 129.6 (s, C-5), 131.7 (d, C-3', C-5'), 132.7 (s, C-1'), 154.2 (s, C-8a), 154.6 (s, C-3). EI: m/z (%) 510-508 (M^+, 8), 323 (12), 185 (54), 183 (90), 157 (29), 155 (12), 85 (13), 76 (17), 71 (30), 69 (26), 57 (100), 55 (56), 43 (55), 42 (21), 41 (89), 39 (19). ESI: *m/z* 531.6 (M + Na^+).

8-(4-Chlorophenyl)-5-methyl-8-(pentadecyloxy)-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (12a). ^{1}H NMR: δ 0.85 (3H, t, *J* = 6.6 Hz, CH_3), 1.23 (24H, m, 12xCH_2), 1.46-1.56 (2H, m, CH_2), 2.40 (3H, d, *J* = 1.3 Hz, 5-CH_3), 3.32 (1H, m, OCH_2), 3.53 (1H, m, OCH_2), 6.21 (1H, q, *J* = 1.3 Hz, H-6), 7.58 (4H, m, H-Ar). ^{13}C NMR: δ 13.8 (q, CH_3), 16.3 (q, 5-CH_3), 22.0 (t, CH_2), 25.2 (t, CH_2), 28.5 (t, 2xCH_2), 28.6 (t, CH_2), 28.8 (t, 2xCH_2), 28.9 (t, 5xCH_2), 31.2 (t, CH_2), 64.5 (t, OCH_2), 82.0 (s, C-8), 103.4 (d, C-6), 128.7 (d, C-3', C-5'), 129.3 (d, C-2', C-6'), 129.6 (s, C-5), 132.3 (s, C-1'), 134.6 (s, C-4'), 154.2 (s, C-8a), 154.6 (s, C-3). ESI: *m/z* 529.6 (M + Na^+).

8-(4-Bromophenyl)-5-methyl-8-(pentadecyloxy)-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (12b). ^{1}H NMR: δ 0.85 (3H, t, *J* = 6.7 Hz, CH_3), 1.23 (24H, m, 12xCH_2), 1.47-1.59 (2H, m, CH_2), 2.39 (3H, d, *J* = 1.3 Hz, 5-CH_3), 3.32 (1H, m, OCH_2), 3.52 (1H, m, OCH_2), 6.21 (1H, q, *J* = 1.3 Hz, H-6), 7.52 (2H, m, part AA' of the AA'XX' system, H-Ar), 7.70 (2H, m, part XX' of the AA'XX' system, H-Ar). ^{13}C NMR: δ 13.8 (q, CH_3), 16.4 (q, 5-CH_3), 22.0 (t, CH_2), 25.2 (t, CH_2), 28.5 (t, 2xCH_2), 28.6 (t, CH_2), 28.8 (t, 2xCH_2), 28.9 (t, 5xCH_2), 31.2 (t, CH_2), 64.5 (t, OCH_2), 82.1 (s, C-8), 103.4 (d, C-6), 123.3 (s, C-4'), 129.5 (d, C-2', C-6'), 129.6 (s, C-5), 131.7 (d, C-3', C-5'), 132.7 (s, C-1'), 154.2 (s, C-8a), 154.6 (s, C-3). ESI: *m/z* 573.6 (M + Na^+).

8-(4-Chlorophenyl)-5-methyl-8-(octadecyloxy)-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (13a). ^{1}H NMR: δ 0.85 (3H, t, *J* = 6.8 Hz, CH_3), 1.23 (30H, m, 15xCH_2), 1.47-1.59 (2H, m, CH_2), 2.39 (3H, d, *J* = 1.2 Hz, 5-CH_3), 3.32 (1H, m, OCH_2), 3.53 (1H, m, OCH_2), 6.22 (1H, q, *J* = 1.2 Hz, H-6), 7.58 (4H, m, H-Ar). ^{13}C NMR: δ 13.9 (q, CH_3), 16.4 (q, 5-CH_3), 22.0 (t, CH_2), 25.2 (t, CH_2), 28.5 (t, 2xCH_2), 28.6 (t, CH_2), 28.8 (t, 3xCH_2), 28.9 (t, 7xCH_2), 31.2 (t, CH_2), 64.5 (t, OCH_2), 82.0 (s, C-8), 103.4 (d, C-6), 128.7 (d, C-3', C-5'), 129.3 (d, C-2', C-6'), 129.6 (s, C-5), 132.3 (s, C-1'), 134.6 (s, C-4'), 154.3 (s, C-8a), 154.6 (s, C-3). ESI: *m/z* 571.7 (M + Na^+).

8-(4-Bromophenyl)-5-methyl-8-(octadeciloxy)-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (13b). ^{1}H NMR: δ 0.85 (3H, t, *J* = 6.8 Hz, CH_3), 1.23 (30H, m, 15xCH_2), 1.47-1.58 (2H, m, CH_2), 2.39 (3H, d, *J* = 1.2 Hz, 5-CH_3), 3.32 (1H, m, OCH_2), 3.53 (1H, m, OCH_2), 6.21 (1H, q, *J* = 1.2 Hz, H-6), 7.52 (2H, m, part AA' of the AA'XX' system, H-Ar), 7.70 (2H, m, part XX' of the AA'XX' system, H-Ar). ^{13}C NMR: δ 13.9 (q, CH_3), 16.4 (q, 5-CH_3), 22.1 (t, CH_2), 25.3 (t, CH_2), 28.6 (t, 2xCH_2), 28.7 (t, CH_2), 28.9 (t, 3xCH_2), 29.0 (t, 7xCH_2), 31.2 (t, CH_2), 64.6 (t, OCH_2), 82.1 (s, C-8), 103.4 (d, C-6), 123.3 (s, C-4'), 129.6 (d, C-2', C-6'), 129.6 (s, C-5), 131.7 (d, C-3', C-5'), 132.8 (s, C-1'), 154.2 (s, C-8a), 154.6 (s, C-3). ESI: *m/z* 615.7 (M + Na^+).

8-(4-Chlorophenyl)-8-isopropoxy-5-methyl-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (14a). ^{1}H NMR: δ 1.01 (3H, d, *J* = 6.1 Hz, CH_3), 1.15 (3H, d, *J* = 6.1 Hz, CH_3), 2.39 (3H, d, *J* = 1.2 Hz, 5-CH_3), 3.91 (1H, m, O-CH), 6.24 (1H, q, *J* =1.2 Hz, H-6), 7.56 (2H, m, part AA' of the AA'XX' system, H-Ar), 7.65 (2H, m, part XX' of the AA'XX' system, H-Ar). ^{13}C NMR: δ 16.1 (q, 5-CH_3), 23.1 (q, 2xCH_3), 69.6 (d, OCH), 81.8 (s, C-8), 103.9 (d, C-6), 128.2 (d, C-3', C-5'), 128.3 (s, C-5), 129.4 (d, C-

2', C-6'), 133.5 (s, C-1'), 134.4 (s, C-4'), 154.1 (s, C-8a), 154.4 (s, C-3). EI: m/z (%) 340-338 (M^+, 17), 199 (17), 157 (66), 139 (100), 111 (47), 75 (12), 71 (10), 45 (13), 43 (52), 41 (18). ESI: *m/z* 361.3 (M + Na^+).

8-(4-Bromophenyl)-8-isopropoxy-5-methyl-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (14b). ^{1}H NMR: δ 1.01 (3H, d, *J* = 6.3 Hz, CH_3), 1.15 (3H, d, *J* = 6.3 Hz, CH_3), 2.40 (3H, d, *J* = 1.0 Hz, 5-CH_3), 3.92 (1H, m, OCH), 6.25 (1H, q, *J* = 1.0 Hz, H-6), 7.59 (2H, m, part AA' of the AA'XX' system, H-Ar), 7.70 (2H, m, part XX' of the AA'XX' system, H-Ar). ^{13}C NMR: δ: 16.2 (q, 5-CH_3), 23.2 (q, 2xCH_3), 69.7 (d, OCH), 82.0 (s, C-8), 103.9 (d, C-6), 123.2 (s, C-4'), 129.4 (s, C-5), 129.7 (d, C-2', C-6'), 131.2 (d, C-3', C-5'), 134.0 (s, C-1'), 154.1 (s, C-8a), 154.5 (s, C-3). EI: m/z (%) 384-382 (M^+, 7), 199 (18), 185-183 (100), 157 (46), 155 (26), 113 (30), 76 (30), 75 (12), 45 (17), 43 (66), 42 (13), 41 (32), 39 (16). ESI: *m/z* 405.3 (M + Na^+).

8-(Allyloxy)-8-(4-chlorophenyl)-5-methyl-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (15a). ^{1}H NMR: δ 2.41 (3H, d, *J* = 1.0 Hz, 5-CH_3), 3.93 (1H, m, OCH_2), 4.10 (1H, m, OCH_2), 5.23 (2H, m, CH_2), 5.89 (1H, m, CH), 6.21 (1H, q, *J* = 1.0 Hz, H-6), 7.60 (4H, m, H-Ar). ^{13}C NMR: δ 16.5 (q, 5-CH_3), 65.9 (t, OCH_2), 82.1 (s, C-8), 103.3 (d, C-6), 117.5 (t, =CH_2), 128.8 (d, C-3', C-5'), 129.3 (d, C-2', C-6'), 129.6 (s, C-5), 132.3 (s, C-1'), 133.2 (d, CH=), 134.7 (s, C-4'), 154.0 (s, C-8a), 154.6 (s, C-3). EI: m/z (%) 338-336 (M^+, 6), 153 (21), 141 (35), 139 (100), 113 (24), 111 (57), 75 (33), 45 (20), 41 (79), 39 (34). ESI: *m/z* 359.3 (M + Na^+).

8-(Allyloxy)-8-(4-bromophenyl)-5-methyl-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (15b). ^{1}H NMR: δ 2.40 (3H, d, *J* = 1.2 Hz, 5-CH_3), 3.93 (1H, m, OCH_2), 4.10 (1H, m, OCH_2), 5.23 (2H, m, CH_2), 5.88 (1H, m, CH), 6.21 (q, 1H, *J* = 1.2 Hz, H-6), 7.54 (2H, m, part AA' of the AA'XX' system, H-Ar), 7.72 (2H, m, part XX' of the AA'XX' system, H-Ar). ^{13}C NMR: δ 16.2 (q, 5-CH_3), 65.7 (t, OCH_2), 82.1 (s, C-8), 103.1 (d, C-6), 117.2 (t, CH_2), 123.2 (s, C-4'), 129.3 (d, C-2', C-6'), 129.4 (s, C-5), 131.5 (d, C-3', C-5'), 132.6 (s, C-1'), 132.9 (d, CH), 153.8 (s, C-8a), 154.3 (s, C-3). EI: m/z (%) 382-380 (M^+, 12), 197 (35), 185 (100), 157 (56), 155 (47), 153 (58), 75 (20), 50 (25), 45 (54), 41 (54), 39 (32). ESI: *m/z* 403.2 (M + Na^+).

8-(4-Chlorophenyl)-5-methyl-8-[(*E*)-2-pentenyloxy]-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (16a). ^{1}H NMR: δ 0.94 (3H, t, *J* = 7.3 Hz, CH_3), 2.01 (2H, m, CH_2), 2.41 (3H, d, *J* = 1.0 Hz, 5-CH_3), 3.86 (1H, m, OCH_2), 4.05 (1H, m, OCH_2), 5.44-5.53 (1H, m, CH); 5.68-5.78 (1H, m, CH); 6.21 (1H, q, *J* = 1.0 Hz, H-6), 7.59 (4H, m, H-Ar). ^{13}C NMR: δ 13.0 (q, CH_3), 16.5 (q, 5-CH_3), 24.6 (t, CH_2), 66.0 (t, OCH_2), 82.0 (s, C-8), 103.4 (d, C-6), 123.6 (d, CH), 128.8 (d, C-3', C-5'), 129.4 (d, C-2', C-6'), 129.5 (s, C-5), 132.4 (s, C-1'), 134.6 (s, C-4'), 136.4 (d, CH), 154.0 (s, C-8a), 154.6 (s, C-3). ESI: *m/z* 387.3 (M + Na^+).

8-(4-Bromophenyl)-5-methyl-8-[(*E*)-2-pentenyloxy]-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (16b). ^{1}H NMR: δ 0.94 (3H, t, *J* = 7.3 Hz, CH_3), 2.01 (2H, m, CH_2), 2.40 (3H, d, *J* = 1.2 Hz, 5-CH_3), 3.86 (1H, m, OCH_2), 4.05 (1H, m, OCH_2), 5.44-5.53 (1H, m, CH); 5.68-5.77 (1H, m, CH); 6.21 (1H, q, *J* = 1.2 Hz, H-6), 7.53 (2H, m, part AA' of the AA'XX' system, H-Ar), 7.71 (2H, m, part XX' of the AA'XX' system, H-Ar). ^{13}C NMR: δ 13.0 (q, CH_3), 16.5 (q, 5-CH_3), 24.6 (t, CH_2), 66.0 (t, OCH_2), 82.0 (s, C-8), 103.4 (d, C-6), 123.3 (s, C-4'), 123.6 (d, CH), 129.5 (s, C-5), 129.6 (d, C-2', C-6'), 131.7 (d, C-3', C-5'), 132.9 (s, C-1'), 136.4 (d, CH), 154.0 (s, C-8a), 154.6 (s, C-3). ESI: *m/z* 431.3 (M + Na^+).

8-(4-Chlorophenyl)-5-methyl-8-[(*Z*)-2-pentenyloxy]-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (17a). ^{1}H NMR: δ 0.89 (3H, t, *J* = 7.3 Hz, CH_3), 1.96 (2H, m, CH_2), 2.40 (3H, d, *J* = 1.0 Hz, 5-CH_3), 3.95 (1H, m, OCH_2), 4.12 (1H, m, OCH_2), 5.39-5.50 (1H, m, CH); 5.52-5.64 (1H, m, CH); 6.21 (1H, q, *J* = 1.0 Hz, H-6), 7.59 (4H, m, H-Ar). ^{13}C NMR: δ 13.9 (q, CH_3), 16.5 (q, 5-CH_3), 20.4 (t, CH_2), 60.9 (t, OCH_2), 82.0 (s, C-8), 103.3 (d, C-6), 123.4 (d, CH), 128.8 (d, C-3', C-5'), 129.4 (d, C-2', C-6'), 129.7 (s, C-5), 132.2 (s, C-1'), 134.7 (s, C-4'), 136.1 (d, CH), 154.1 (s, C-8a), 154.6 (s, C-3). ESI: *m/z* 387.3 (M + Na^+).

8-(4-Bromophenyl)-5-methyl-8-[(*Z*)-2-pentenyloxy]-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (17b). ^{1}H NMR: δ 0.89 (3H, t, *J* = 7.5 Hz, CH_3), 1.95 (2H, m, CH_2), 2.40 (3H, d, *J* = 1.2 Hz, 5-CH_3),

3.95 (1H, m, OCH_2), 4.12 (1H, m, OCH_2), 5.41-5.49 (1H, m, CH); 5.54-5.63 (1H, m, CH); 6.23 (1H, q, *J* = 1.2 Hz, H-6), 7.53 (2H, m, part AA' of the AA'XX' system, H-Ar), 7.72 (2H, m, part XX' of the AA'XX' system, H-Ar). ^{13}C NMR: δ 13.9 (q, CH_3), 16.5 (q, 5-CH_3), 20.4 (t, CH_2), 60.9 (t, OCH_2), 82.1 (s, C-8), 103.3 (d, C-6), 123.3 (d, CH), 123.4 (s, C-4'), 129.6 (d, C-2', C-6'), 129.7 (s, C-5), 131.8 (d, C-3', C-5'), 132.6 (s, C-1'), 136.1 (d, CH), 154.0 (s, C-8a), 154.6 (s, C-3). ESI: *m/z* 431.3 (M + Na^+).

8-(4-Chlorophenyl)-5-methyl-8-[(*Z*)-9-octadecenyloxy]-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (18a). ^{1}H NMR: δ 0.84 (3H, t, *J* = 6.8 Hz, CH_3), 1.23 (22H, m, 11xCH_2), 1.47-1.60 (2H, m, CH_2), 1.90-1.98 (4H, m, 2xCH_2), 2.39 (3H, d, *J* = 1.0 Hz, 5-CH_3), 3.31 (1H, m, OCH_2), 3.52 (1H, m, OCH_2), 5.29-5.35 (2H, m, 2xCH), 6.22 (1H, q, *J* = 1.0 Hz, H-6), 7.58 (4H, m, H-Ar). ^{13}C NMR: δ 13.9 (q, CH_3), 16.4 (q, 5-CH_3), 22.0 (t, CH_2), 25.3 (t, CH_2), 26.5 (t, CH_2), 28.5 (t, CH_2), 28.6 (t, 2xCH_2), 28.7 (t, CH_2), 28.8 (t, 2xCH_2), 28.9 (t, 2xCH_2), 29.1 (t, CH_2), 31.2 (t, CH_2), 31.9 (t, CH_2), 64.5 (t, OCH_2), 82.0 (s, C-8), 103.4 (d, C-6), 128.8 (d, C-3', C-5'), 129.3 (d, C-2', C-6'), 129.6 (s, C-5), 130.0 (d, CH), 130.0 (d, CH), 132.3 (s, C-1'), 134.6 (s, C-4'), 154.3 (s, C-8a), 154.6 (s, C-3). EI: m/z (%) 548-546 (M^+, 12), 281 (37), 279 (52), 252 (14), 235 (17), 201 (15), 157 (46), 139 (100), 111 (28), 110 (11), 97 (25), 95 (18), 85 (11), 83 (60), 81 (17), 71 (11), 69 (47), 55 (77), 43 (58), 42 (12). ESI: *m/z* 569.7 (M + Na^+).

8-(4-Bromophenyl)-5-methyl-8-[(*Z*)-9-octadecenyloxy]-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (18b). ^{1}H NMR: δ 0.84 (t, 3H, *J* = 6.3 Hz, CH_3), 1.23 (m, 22H, 11xCH_2), 1.46-1.56 (2H, m, CH_2), 1.92-2.02 (4H, m, 2xCH_2), 2.39 (3H, d, *J* = 1.0 Hz, 5-CH_3), 3.31 (1H, m, OCH_2), 3.52 (1H, m, OCH_2), 5.29-5.35 (2H, m, 2xCH), 6.21 (1H, q, *J* = 1.0 Hz, H-6), 7.52 (2H, m, part AA' of the AA'XX' system, H-Ar), 7.70 (2H, m, part XX' of the AA'XX' system, H-Ar). ^{13}C NMR: δ 13.9 (q, CH_3), 16.4 (q, 5-CH_3), 22.0 (t, CH_2), 25.3 (t, CH_2), 26.5 (t, CH_2), 28.5 (t, 3xCH_2), 28.6 (t, CH_2), 28.8 (t, 2xCH_2), 28.9 (t, 2xCH_2), 29.0 (t, CH_2), 31.2 (t, CH_2), 31.9 (t, CH_2), 64.5 (t, OCH_2), 82.1 (s, C-8), 103.4 (d, C-6), 123.3 (s, C-4'), 129.5 (d, C-2', C-6'), 129.6 (s, C-5), 130.0 (d, CH), 130.0 (d, CH), 131.7 (d, C-3', C-5'), 132.7 (s, C-1'), 154.2 (s, C-8a), 154.6 (s, C-3). EI: m/z (%) 592-590 (M^+, 1), 183 (13), 110 (30), 109 (18), 97 (22), 95 (22), 82 (37), 69 (66), 68 (21), 67 (63), 57 (25), 55 (32), 43 (100). ESI: *m/z* 613.7 (M + Na^+).

8-(Benzyloxy)-8-(4-chlorophenyl)-5-methyl-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (19a). ^{1}H NMR: δ 2.34 (3H, d, *J* = 1.1 Hz, 5-CH_3), 4.41 (1H, m, part A of the system AB, OCH_2), 4.70 (1H, m, part B of the system AB, OCH_2), 6.19 (1H, q, *J* = 1.1 Hz, H-6), 7.28-7.39 (5H, m, H-Ar), 7.60 (2H, m, part AA' of the AA'XX' system, H-Ar), 7.68 (2H, m, part XX' of the AA'XX' system, H-Ar). ^{13}C NMR: δ 16.4 (q, 5-CH_3), 66.8 (t, OCH_2), 82.2 (s, C-8), 103.4 (d, C-6), 127.8 (d, C-2", C-6" or C-3", C-6"), 127.9 (d, C-4"), 128.3 (d, C-3", C-5" or C-2", C-6"), 128.9 (d, C-3', C-5'), 129.4 (d, C-2', C-6'), 129.6 (s, C-5), 132.2 (s, C-1'), 134.7 (s, C-4'), 136.2 (s, C-1"), 153.9 (s, C-8a), 154.5 (s, C-3). EI: m/z (%) 388-386 (M^+, 1), 139 (17), 111 (12), 91 (100). ESI: *m/z* 409.3 (M + Na^+).

8-(Benzyloxy)-8-(4-bromophenyl)-5-methyl-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (19b). ^{1}H NMR: δ 2.34 (3H, d, *J* = 1.3 Hz, 5-CH_3), 4.41 (1H, m, part A of the system AB, OCH_2), 4.70 (1H, m, part B of the system AB, OCH_2), 6.19 (1H, q, *J* = 1.3 Hz, H-6), 7.27-7.39 (5H, m, H-Ar), 7.60 (2H, m, part AA' of the AA'XX' system, H-Ar), 7.74 (2H, m, part XX' of the AA'XX' system, H-Ar). ^{13}C NMR: δ 16.1 (q, 5-CH_3), 66.7 (t, OCH_2), 82.2 (s, C-8), 103.2 (d, C-6), 123.3 (s, C-4'), 127.6 (d, C-2", C-6" or C-3", C-5"), 127.8 (d, C-4"), 128.2 (d, C-3", C-5" or C-2", C-6"), 129.5 (d, C-2', C-6'), 129.5 (s, C-5), 131.6 (d, C-3', C-5'), 132.6 (s, C-1'), 136.1 (s, C-1"), 153.8 (s, C-8a), 154.3 (s, C-3). EI: m/z (%) 432-430 (M^+, 1), 185 (11), 91 (100), 65 (13). ESI: *m/z* 453.3 (M + Na^+).

8-(4-Chlorophenyl)-8-(cyclohexylmethoxy)-5-methyl-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (20a). ^{1}H-NMR: δ 0.81-0.98 (2H, m, CH_2), 1.02-1.28 (3H, m, CH and CH_2), 1.47-1.71 (6H, m, 3xCH_2), 2.39 (3H, d, *J* = 1.2 Hz, 5-CH_3), 3.11 (1H, m, OCH_2), 3.36 (1H, m, OCH_2), 6.21 (1H, q, *J* = 1.2 Hz, H-6), 7.58 (4H, m, H-Ar). ^{13}C-NMR: δ 16.3 (q, 5-CH_3), 25.1 (t, 2xCH_2), 25.9 (t, CH_2), 29.1 (t, 2xCH_2), 36.9 (d, CH), 69.4 (t, OCH_2), 81.9 (s, C-8), 103.5 (d, C-6), 128.8 (d, C-3', C-5'), 129.3 (d, C-2', C-6'), 129.8 (s, C-5), 132.2 (s, C-1'), 134.6 (s, C-4'), 154.3 (s, C-8a), 154.6 (s, C-3). ESI: *m/z* 415.4 (M + Na^+).

8-(4-Bromophenyl)-8-(cyclohexylmethoxy)-5-methyl-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (20b). ^{1}H NMR: δ 0.81-0.97 (2H, m, CH_2), 1.02-1.29 (3H, m, CH and CH_2), 1.48-1.70 (6H, m, 3xCH_2), 2.39 (3H, d, J = 1.0 Hz, 5-CH_3), 3.11 (1H, m, OCH_2), 3.35 (1H, m, OCH_2), 6.21 (1H, q, J = 1.0 Hz, H-6), 7.51 (2H, m, part AA' of the AA'XX' system, H-Ar), 7.71 (2H, m, part XX' of the AA'XX' system, H-Ar). ^{13}C NMR: δ 16.4 (q, 5-CH_3), 25.1 (t, 2xCH_2), 25.9 (t, CH_2), 29.1 (t, 2xCH_2), 36.9 (d, CH), 69.4 (t, OCH_2), 82.0 (s, C-8), 103.4 (d, C-6), 123.3 (s, C-4'), 129.6 (d, C-2', C-6'), 129.8 (s, C-5), 131.7 (d, C-3', C-5'), 132.6 (s, C-1'), 154.3 (s, C-8a), 154.6 (s, C-3). ESI: *m/z* 459.4 ($M + Na^+$).