Supporting Information

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Chemical Constituents and Biological Activities of *Strobilanthes crispus* L.

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Fresh leaves (3 kg) were air-dried for 2 weeks at room temperature (27°C). The dried leaves (1 kg) were powdered and macerated sequentially in hexane, dichloromethane and methanol. Each of the different extractions was performed at room temperature a total of three times (3 x 5 L), 24 h each time. All extracts after filtration were evaporated *in vacuo* using a rotary evaporator to give 10 g (0.33% w/w of fresh leaves), 15 g (0.50% w/w of fresh leaves) and 12 g (0.40% w/w of fresh leaves) of hexane, dichloromethane and methanol extracts, respectively.

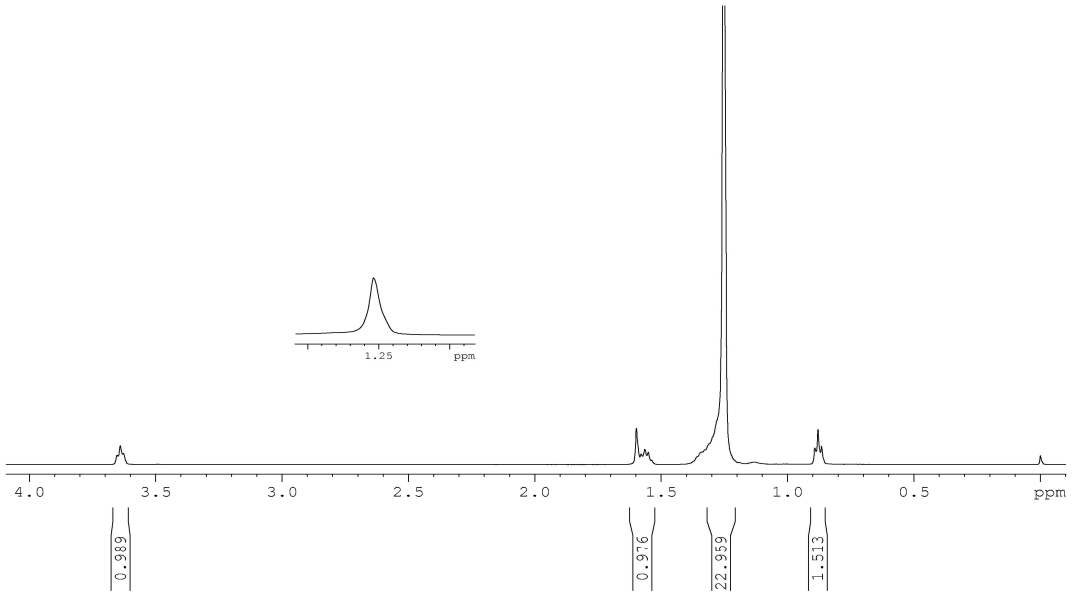
The hexane extract (10 g) was fractionated on a silica gel column, eluting with hexane-$CHCl_3$ (1:0→0:1 v/v), to yield five major fractions (KA1-KA5). Fractions KA1 (yellow oil, 0.50 g), KA2 (yellow oil, 0.4 g) and KA3 (white solid, 0.2 g) were separately rechromatographed over a silica gel column, eluting with hexane-CH_2Cl_2 (8:2 v/v), hexane-CH_2Cl_2 (9:1 v/v) and hexane-CH_2Cl_2 (5:5 v/v), to afford **(1)** (10 mg, 3.3×10^{-4}% w/w), **(2)** (15 mg, 5.0×10^{-4}% w/w) and **(3)** (10 mg, 3.3×10^{-4}% w/w), respectively.

The dichloromethane (DCM) extract (15 g) was subjected to silica gel CC, eluting with hexane-EtOAc-MeOH (1:0:0 → 0:0:1 v/v/v), to give 10 major fractions (KB1 to KB10). Rechromatography of fraction KB2 (yellow oil, 0.7 g) over silica gel using hexane-$CHCl_3$ (8:2 v/v) afforded **(4)** (4 mg, 1.7×10^{-4}% w/w). Rechromatography of fraction KB3 (yellow oil, 2.0 g) over silica gel eluting with hexane-$CHCl_3$ (1:0 →5:5 v/v) yielded three sub-fractions (KB3-1-KB3-3). **(5)** (15 mg, 5.0×10^{-4}% w/w) and **(6)** (10 mg, 3.3×10^{-4}% w/w) were isolated by silica gel CC of sub-fractions KB3-2 (0.2 g) and KB3-3 (0.5 g) using hexane-$CHCl_3$ (8:2 v/v) and (7:3 v/v), respectively. Fraction KB4 (green solid, 1.2 g) was subjected to silica gel CC eluting with hexane-$CHCl_3$ (7:3 v/v) yielded **(7)** (20 mg, 6.7×10^{-4}% w/w).

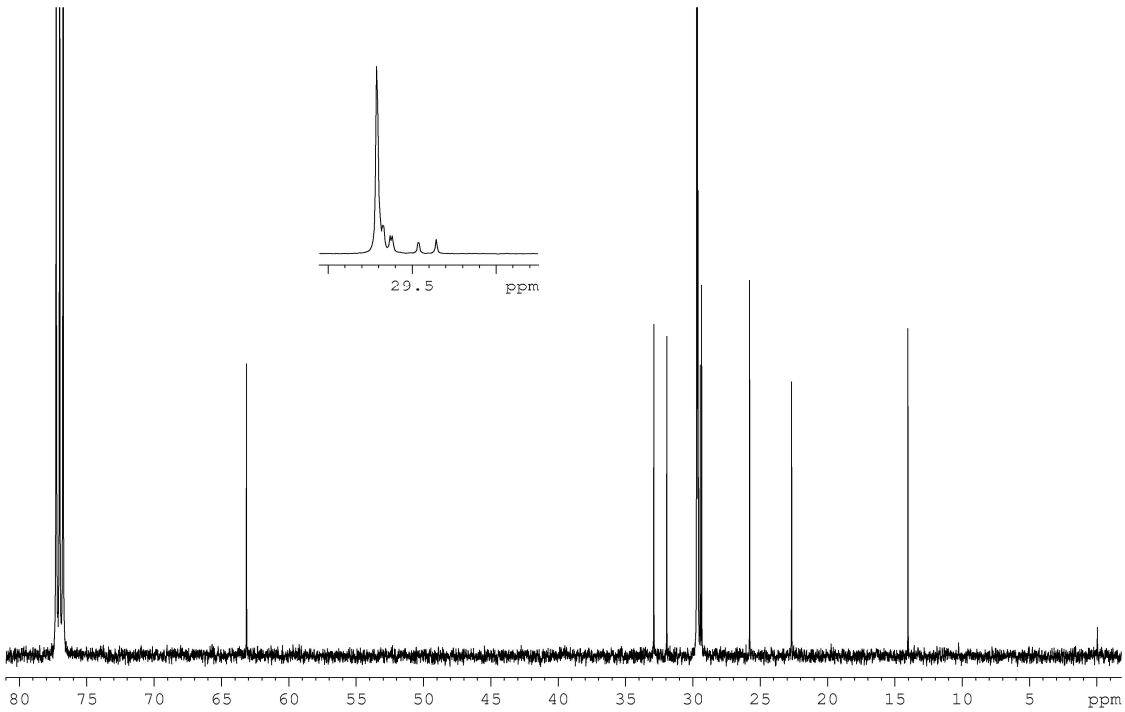
The methanol extract (12 g) was subjected to silica gel CC using hexane-EtOAc-MeOH (1:0:0 → 0:0:1 v/v/v) to give five major fractions (KC1-KC5). Fraction KC2 (green solid, 2.2 g) was further fractionated over a silica gel column to give sub-fractions (KC2-1-KC2-5). Repeated silica gel CC of KC2-2 (0.1 g) yielded **(8)** (4 mg, 1.3×10^{-4}% w/w). Fractionation of KC3 (green solid, 2.5 g) afforded three sub-fractions (KC3-1-KC3-3). Sub-fraction KC3-2 (0.3 g) afforded **(9)** (5 mg, 1.7×10^{-4}% w/w) after silica gel CC using CH_3Cl-EtOAc (7:3 v/v).

Trans-esterification of (**4**) and (**7**): **(4)** (2 mg) and **(7)** (8 mg) were separately refluxed with 2 mL 14% boron trifluoride-methanol reagent for 30 minutes on an oil bath (80°C). After cooling below room temperature, the suspension was transferred to a 5 mL test tube and extracted with 4 mL of reagent grade hexane. The organic layer, which contained the methyl esters, was analyzed by capillary GC and GC-MS. The identity of the methyl esters were confirmed comparison of retention indice and mass spectra with those of authentic substances.

1-Heptacosanol **(1)**: white powder; mp 81-82°C; EIMS *m/z* (rel. int. %): 396 M^+ (1), 392 (3), 218 (6), 153 (8), 139 (12), 125 (28), 111 (51), 97 (92), 83 (95), 57 (100), 43 (86); IR υ_{max} (KBr cm^{-1}): 3296, 2918, 2849, 1463, 1062, 719; ^{1}H NMR (500 MHz, $CDCl_3$): δ_H 3.64 (2H, t, J = 6.3 Hz, H-1), 1.57 (2H, m, H-2), 1.25 (45H, br s, H-3-26), 0.88 (3H, t, J = 6.6 Hz, H-27); ^{13}C NMR (125 MHz, $CDCl_3$): δ_C 63.1 (C-1), 32.9 (C-2), 31.9 (C-3), 29.4-29.7 (C-4-24), 25.8 (C-25), 22.7 (C-26), 14.1 (C-27).

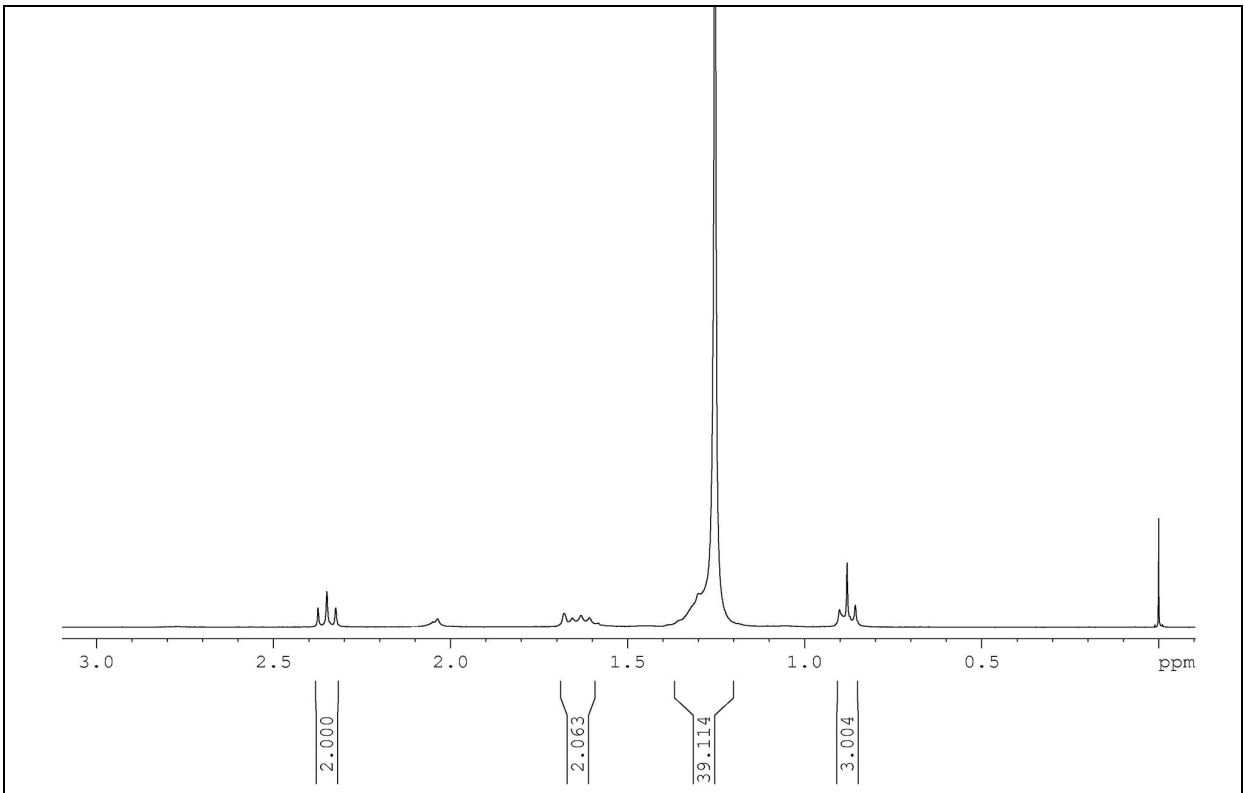


S1. ^{1}H NMR spectrum of 1-heptacosanol **(1)** in $CDCl_3$ (500 MHz)

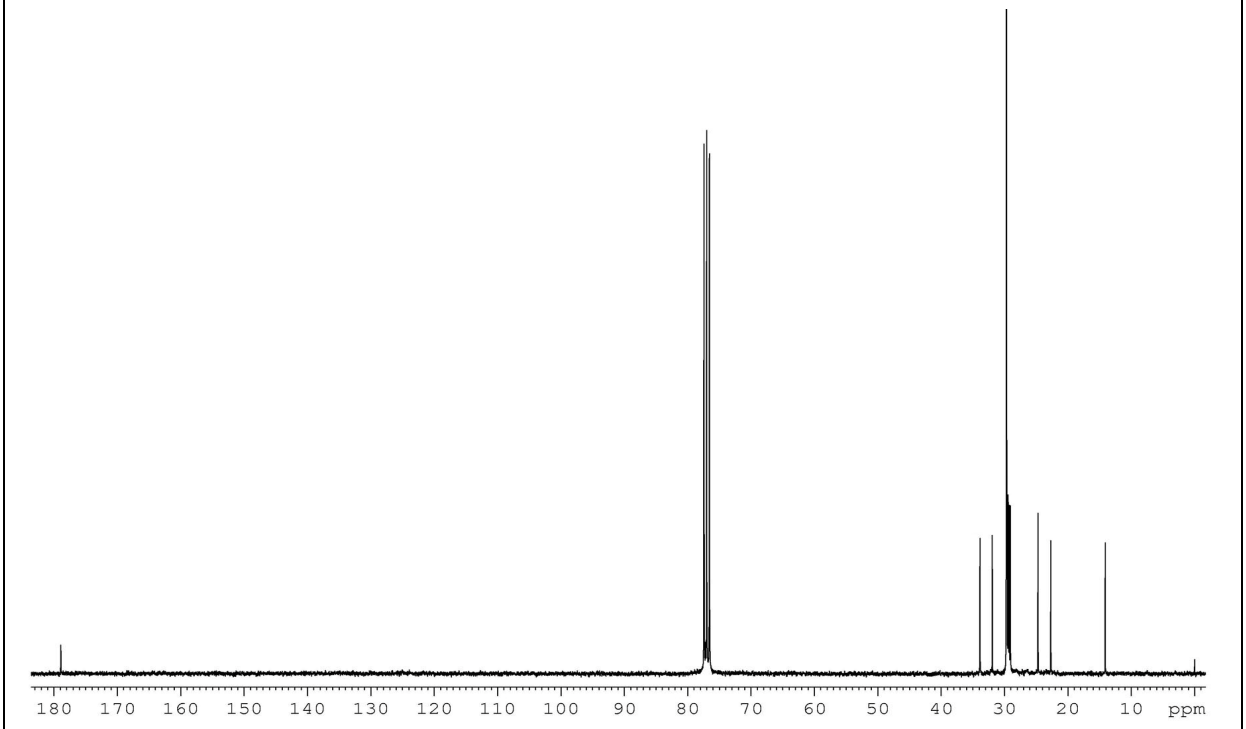


S2. ^{13}C NMR spectrum of 1-heptacosanol **(1)** in $CDCl_3$ (125 MHz)

Tetracosanoic acid **(2)**: white powder; mp 78-79°C; EIMS *m/z* (rel. int. %): 368 M^+ (11), 340 (22), 222 (32), 129 (31), 100 (65), 81 (100), 57 (53), 43 (56); IR υ_{max} (KBr cm^{-1}): 3415, 2918, 2849, 1709, 1463, 720; ^1H NMR (400 MHz, $CDCl_3$): δ_H 2.35 (2H, t, J = 7.5 Hz, H-2), 1.63 (2H, m, H-3), 1.25 (40H, br s, H-4-23), 0.88 (3H, t, J = 6.7 Hz, H-24); ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 179.0 (C-1), 34.1 (C-2), 32.1 (C-3), 29.3-29.9 (C-4-21), 24.9 (C-22), 22.9 (C-23), 14.3 (C-24).

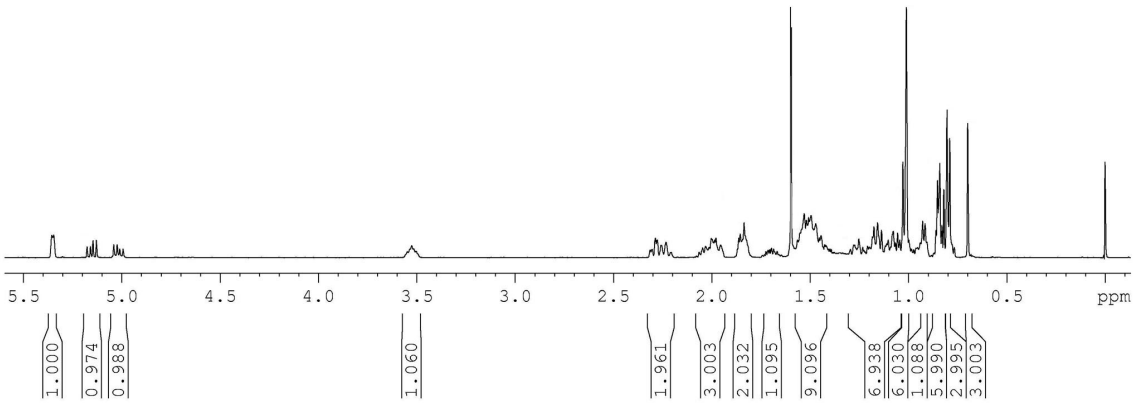


S3. ^1H NMR spectrum of tetracosanoic acid **(2)** in $CDCl_3$ (400 MHz)

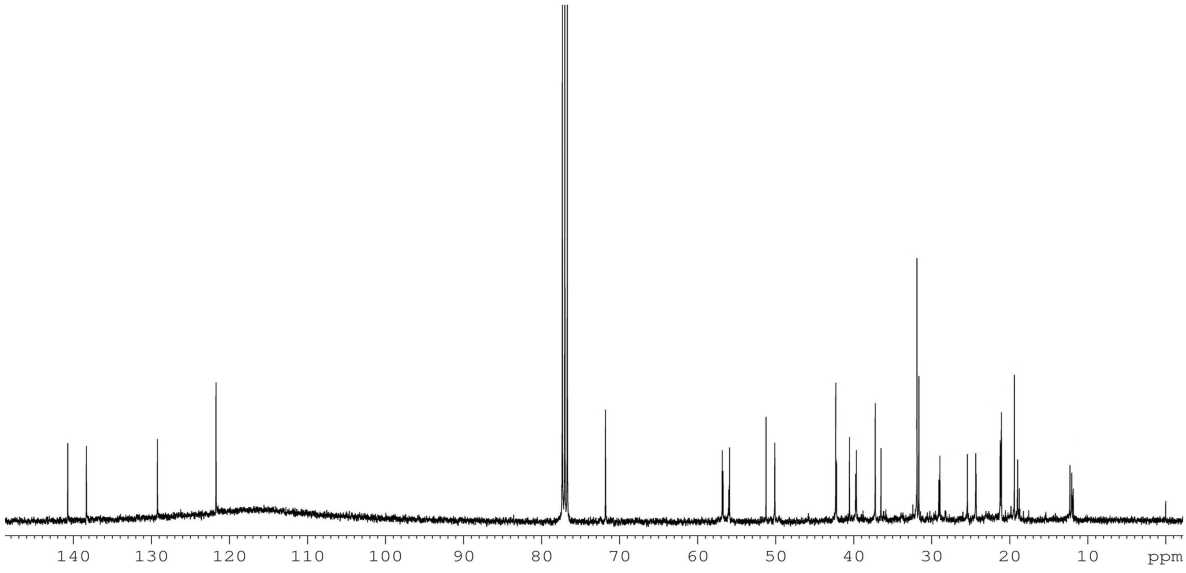


S4. ^{13}C NMR spectrum of tetracosanoic acid **(2)** in $CDCl_3$ (100 MHz)

Stigmasterol (stigmasta-5,22(*E*)-dien-3β-ol) **(3)**: white crystalline solid; mp 169-171°C; EIMS *m/z* (rel. int. %): 412 M^+ (58), 394 (5), 369 (9), 351 (17), 329 (10), 300 (25), 274 (17), 273 (16), 255 (50), 145 (48), 138 (13), 105 (54), 55 (100); IR υ_{max} (KBr cm^{-1}): 3437, 2938, 2868, 1639, 1465, 1382, 1051, 959, 800; ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 5.35 (1H, m, H-6), 5.15 (1H, dd, *J* = 15.2, 8.6 Hz, H-22), 5.02 (1H, dd, *J* = 15.2, 8.6 Hz, H-23), 3.52 (1H, m, H-3), 2.31 (1H, m, H-4b), 2.23 (1H, m, H-4a), 2.06 (1H, m, H-20), 2.00 (1H, m, H-12b), 1.96 (1H, m, H-7b), 1.86 (1H, m, H-1b), 1.84 (1H, m, H-2b), 1.72 (1H, m, H-16b), 1.56 (2H, m, H-15b, H-28b), 1.54 (1H, m, H-25), 1.53 (1H, m, H-24), 1.52 (1H, m, H-2a), 1.50 (3H, m, H-7a, H-11a, H-11b), 1.47 (1H, m, H-8), 1.29 (1H, m, H-16a), 1.22 (1H, m, H-28a), 1.18 (1H, m, H-12a), 1.15 (1H, m, H-17), 1.09 (1H, m, H-1a), 1.04 (2H, m, H-14, H-15a, 3H, s, H-21), 1.01 (3H, s, H-19), 0.93 (1H, m, H-9), 0.92 (3H, d, *J* = 5.8 Hz, H-26), 0.83 (3H, br s, H-29), 0.81 (3H, br s, H-27), 0.70 (3H, s, H-18); ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 141.1 (C-5), 138.7 (C-22), 129.6 (C-23), 122.1 (C-6), 72.2 (C-3), 57.2 (C-14), 56.3 (C-17), 51.6 (C-24), 50.5 (C-9), 42.7 (C-4), 42.6 (C-13), 41.0 (C-20), 40.0 (C-12), 37.6 (C-1), 36.6 (C-10), 32.3 (C-8, C-25), 32.0 (C-2, C-7), 28.7 (C-16), 25.8 (C-28), 24.7 (C-15), 21.5 (C-11, C-21, C-26), 19.4 (C-19), 19.2 (C-27), 12.4 (C-29), 12.3 (C-18).

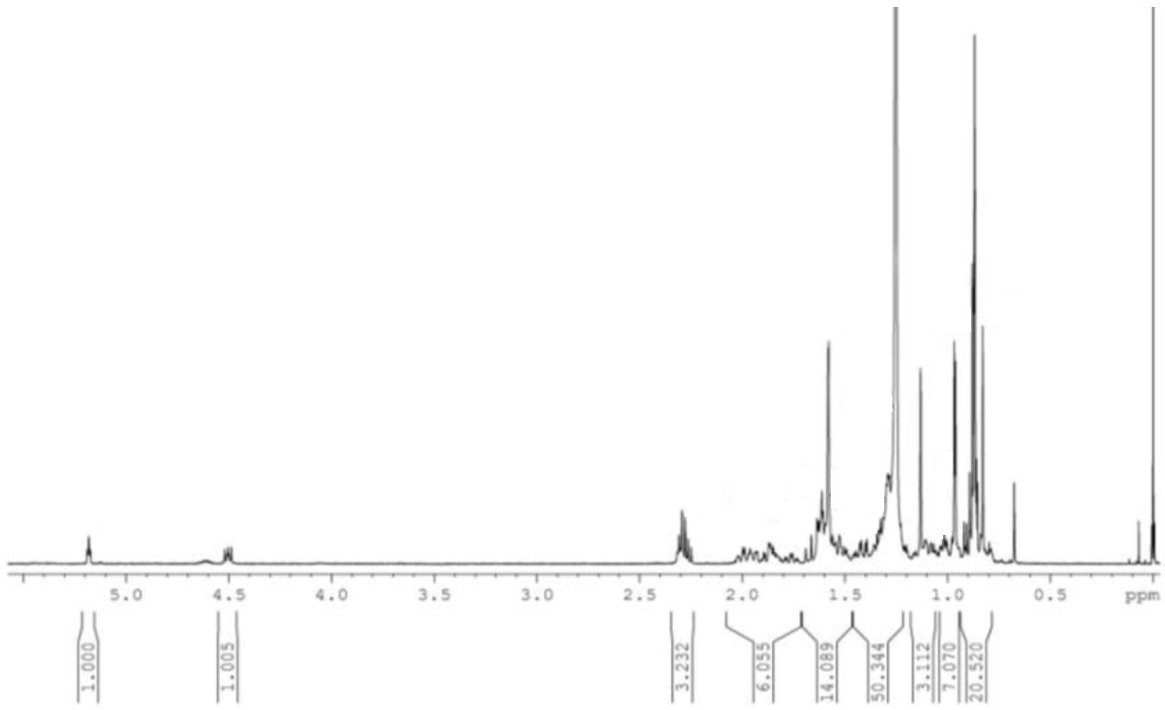


S5. ^{1}H NMR spectrum of stigmasterol **(3)** in $CDCl_3$ (400 MHz)

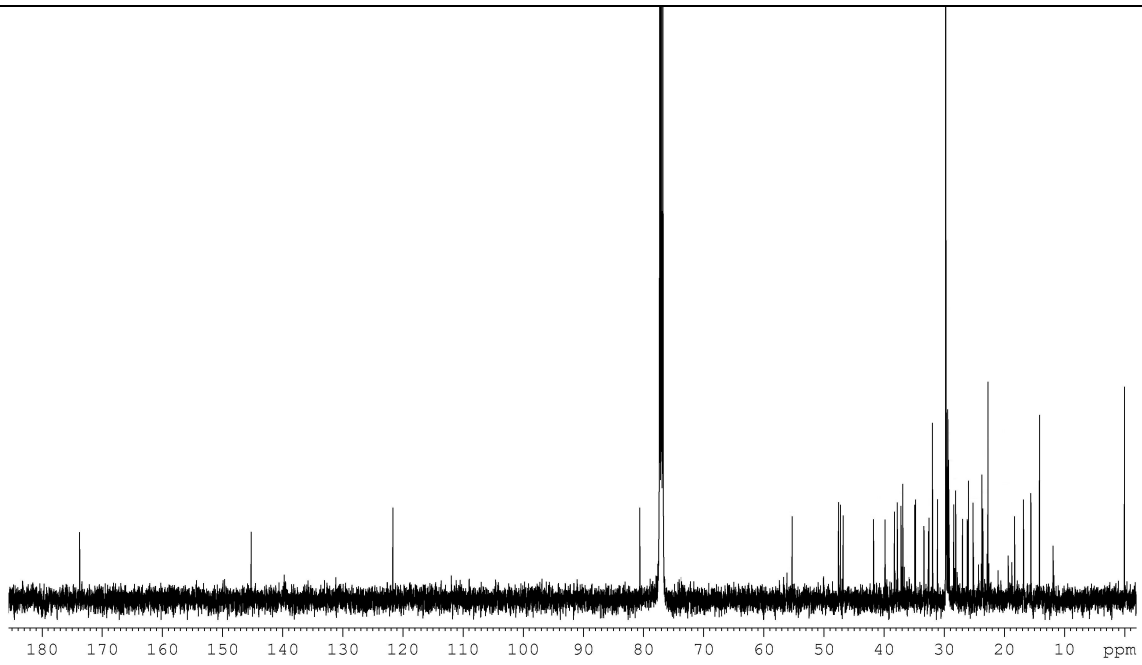


S6. ^{13}C NMR spectrum of stigmasterol **(3)** in $CDCl_3$ (100 MHz)

A mixture of fatty acid esters of *β*-amyrin: *β*-amyrin 3-docosanoate (olean-12-en-3*β*-docosanoate), *β*-amyrin 3-tetracosanoate (olean-12-en-3*β*-tetracosanoate), *β*-amyrin 3-eicosanoate (olean-12-en-3*β*-eicosanoate) and *β*-amyrin 3-tricosanoate (olean-12-en-3*β*- tricosanoate) **(4)**: white powder; mp 202-204°C; EIMS *m/z* (rel. int. %): 425 (2), 409 (6), 368 (35), 218 (100), 207 (6), 203 (23), 189 (10), 57 (21); IR υ_{max} (KBr cm^{-1}): 2917, 2849, 1737, 1473, 1384, 1174, 719; ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 5.18 (1H, m, H-12), 4.50 (1H, t, *J* = 8.0 Hz, H-3), 2.29 (2H, m, CH_2COO), 2.28 (1H, m, H-18), 1.96 (1H, m, H-16b), 1.90 (1H, m, H-11b), 1.87 (2H, m, H-15b, H-19b), 1.84 (1H, m, H-22b), 1.79 (1H, m, H-2b), 1.69 (1H, m, H-9), 1.66 (1H, m, H-1b), 1.61 (1H, m, H-11a), 1.58 (3H, m, H-6b), 1.55 (1H, m, H-22a), 1.53 (1H, m, H-7b), 1.50 (1H, m, H-19a), 1.45 (1H, m, H-16a), 1.39 (2H, m, H-6a, H-21b), 1.33 (1H, m, H-7a), 1.25 (43H, m, H-15a, H-21a, $(CH_2)_{n-1}$, n = 18, 20, 21, 22), 1.21 (1H, m, H-2a), 1.13 (3H, s, H-27), 1.02 (1H, m, H-1a), 0.97 (3H, s, H-26), 0.96 (3H, s, H-25), 0.89 (1H, m, H-5), 0.88 (6H, s, H-23, H-24), 0.87 (9H, s, H-29, H-30, $C\underline{H}_3(CH_2)_{n-1}$, n = 18, 20, 21, 22), 0.83 (3H, s, H-28); ^{13}C NMR (125 MHz, $CDCl_3$): δ_C 173.7 (CO), 145.2 (C-13), 121.7 (C-12), 80.6 (C-3), 55.3 (C-5), 47.6 (C-9), 47.2 (C-18), 46.8 (C-19), 41.7 (C-14), 39.8 (C-8), 38.2 (C-1), 37.8 (C-4), 37.1 (C-22), 37.0 (C-10), 34.7 (C-21), 33.3 (C-29), 32.6 (C-7), 32.5 (C-17), 31.9 ($\underline{C}H_2COO$), 31.1 (C-20), 29.6-29.1 ($(CH_2)_{n-1}$, n = 18, 20, 21, 22), 28.4 (C-15), 28.0 (C-23), 26.9 (C-28), 26.1 (C-16), 26.0 (C-27), 23.7 (C-30), 23.6 (C-2), 23.5 (C-11), 18.3 (C-6), 16.8 (C-24, C-26), 15.6 (C-25), 14.1 ($\underline{C}H_3(CH_2)_{n-1}$, n = 18, 20, 21, 22). Capillary GC and GC-MS analyses of the products of *trans*-esterification of **(4)** indicated that (**4**) was a mixture of predominately *β*-amyrin 3-docosanoate and *β*-amyrin 3-tetracosanoate, with lesser proportions of *β*-amyrin 3-eicosanoate and *β*-amyrin 3-tricosanoate.



S7. ^{1}H NMR spectrum of the mixture of *β*-amyrin 3-docosanoate, *β*-amyrin 3-tetracosanoate, *β*-amyrin 3-eicosanoate and *β*-amyrin 3-tricosanoate **(4)** in $CDCl_3$ (500 MHz)

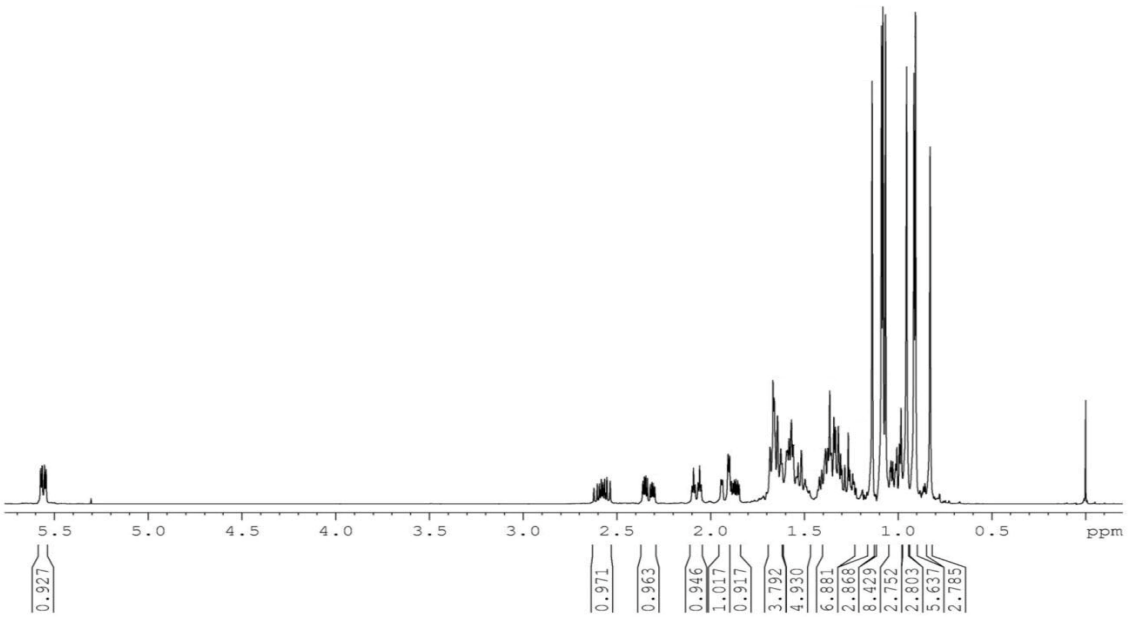


S8. ^{13}C NMR spectrum of the mixture of *β*-amyrin 3-docosanoate, *β*-amyrin 3-tetracosanoate, *β*-amyrin 3-eicosanoate and *β*-amyrin 3-tricosanoate **(4)** in $CDCl_3$ (125 MHz)

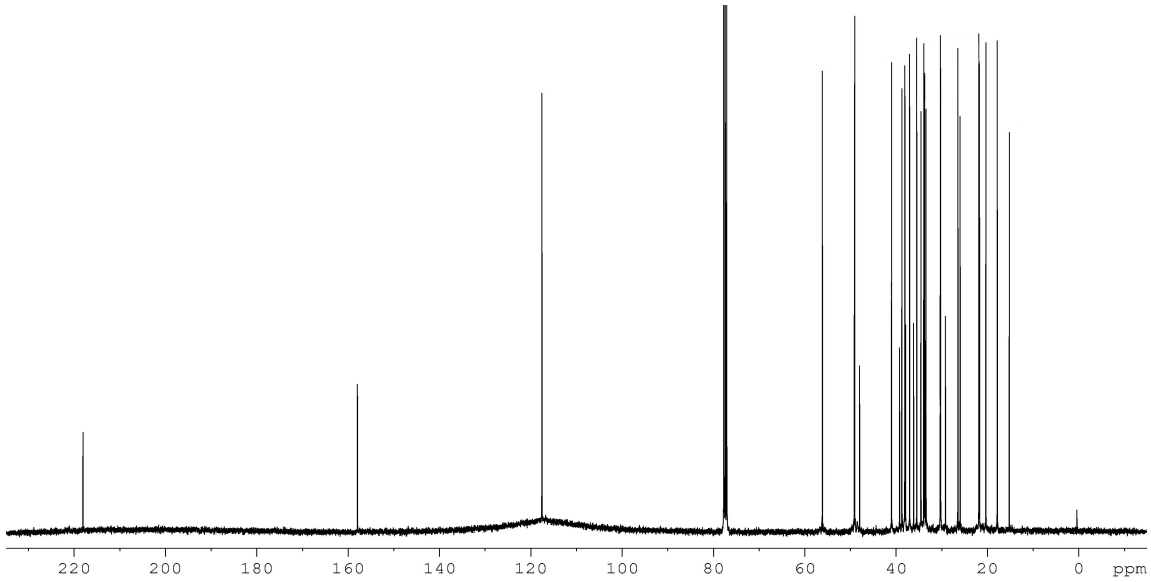
Table 1. GC analysis of *trans*-esterified products of **(4)**

Peak No	RT (min)	%	Compound
1	35.09	16.82	Methyl eicosanoate
2	38.24	38.12	Methyl docosanoate
3	39.67	18.05	Methyl tricosanoate
4	41.13	27.00	Methyl tetracosanoate

Taraxerone (13α-methyl-27-norolean-14-en-3β-one) **(5)**: white crystalline solid; mp 239-240°C; EIMS *m/z* (rel. int. %): 424 M^+ (41), 409 (29), 300 (92), 285 (71), 204 (100), 189 (42), 133 (70), 69 (61); IR υ_{max} (KBr cm^{-1}): 2938, 2863, 1709, 1450, 1376, 1150, 995, 816; ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 5.56 (1H, dd, *J* = 8.2, 3.2 Hz, H-15), 2.58 (1H, m, H-2b), 2.33 (1H, ddd, *J* = 15.9, 6.4, 3.3 Hz, H-2a), 2.08 (1H, m, H-19b), 1.92 (1H, m, H-16b), 1.87 (1H, m, H-1b), 1.68 (1H, m, H-11b), 1.66 (1H, m, H-1a), 1.64 (1H, m, H-7b), 1.62 (1H, m, H-16a), 1.60 (1H, m, H-6b), 1.57 (1H, m, H-7a), 1.54 (1H, m, H-11a), 1.52 (1H, m, H-18), 1.50 (1H, m, H-6a), 1.37 (1H, m, H-19a), 1.34 (1H, m, H-12b), 1.32 (1H, m, H-22b), 1.30 (1H, m, H-22a), 1.27 (2H, m, H-21), 1.14 (3H, s, H-27), 1.09 (3H, s, H-23), 1.08 (3H, s, H-25), 1.07 (3H, s, H-24), 1.04 (1H, m, H-12a), 1.01 (1H, m, H-9), 0.96 (3H, s, H-29), 0.92 (3H, s, H-28), 0.91 (3H, s, H-30), 0.86 (1H, m, H-5), 0.83 (3H, s, H-26); ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 217.9 (C-3), 157.9 (C-14), 117.6 (C-15), 56.2 (C-5), 49.2 (C-18), 49.1 (C-9), 47.9 (C-4), 41.0 (C-19), 39.3 (C-8), 38.7 (C-1), 37.9 (C-13), 38.1 (C-10, C-17), 37.1 (C-16), 36.2 (C-12), 35.5 (C-7), 34.5 (C-2), 33.9 (C-21), 33.7 (C-29), 33.5 (C-22), 30.3 (C-26, C-28), 29.2 (C-20), 26.5 (C-23), 26.0 (C-27), 21.9 (C-24), 21.7 (C-30), 20.4 (C-6), 17.8 (C-11), 15.2 (C-25).

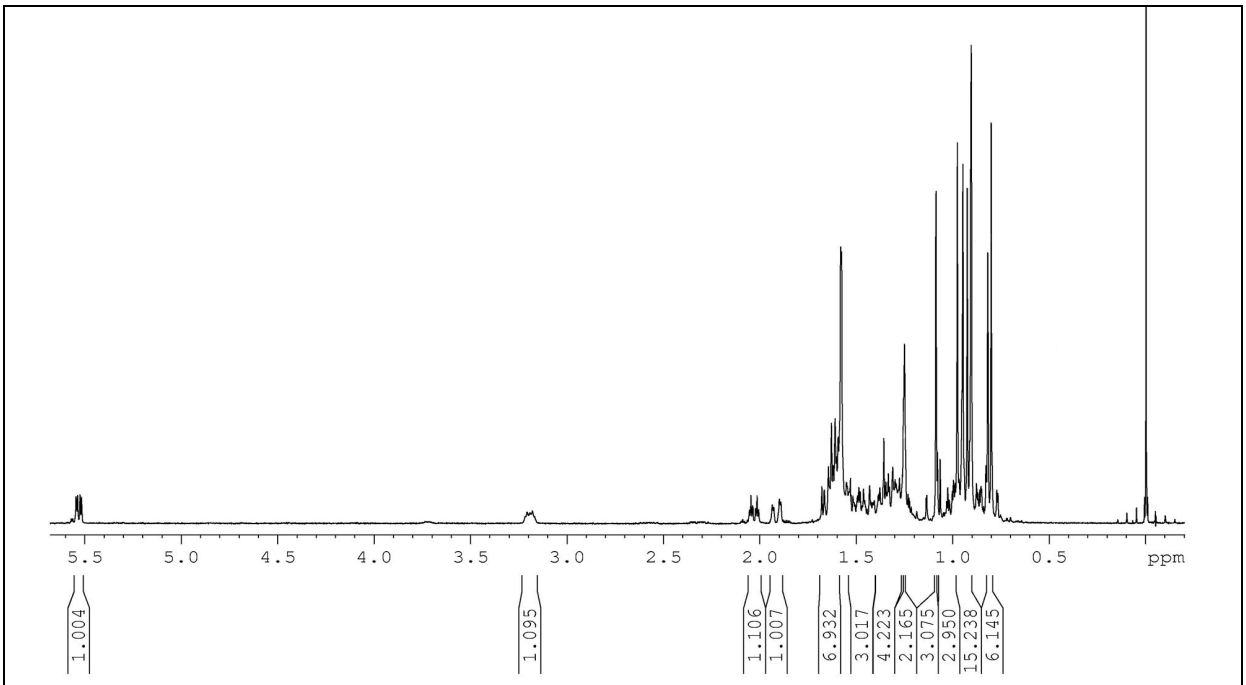


S9. ^{1}H NMR spectrum of taraxerone **(5)** in $CDCl_3$ (400 MHz)

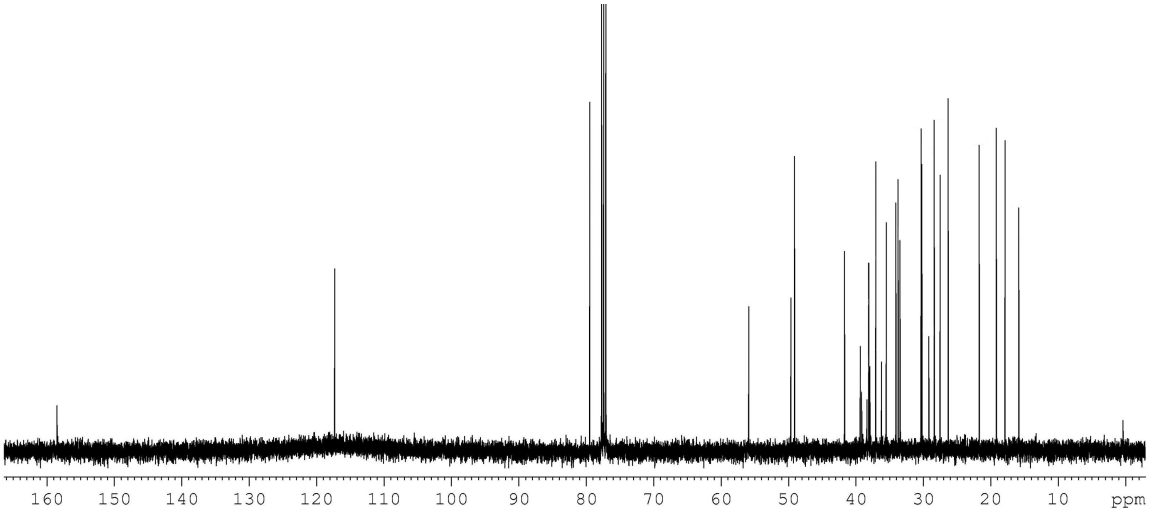


S10. ^{13}C NMR spectrum of taraxerone **(5)** in $CDCl_3$ (100 MHz)

Taraxerol (13α-methyl-27-norolean-14-en-3β-ol) **(6)**: white crystalline solid; mp 276-278°C; EIMS *m/z* (rel. int. %): 426 M^+ (16), 411 (12), 302 (46), 287 (44), 204 (100), 135 (42), 69 (52); IR υ_{max} (KBr cm^{-1}): 3484, 2934, 2856, 1640, 1474, 1376, 1037, 999, 816; ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 5.53 (1H, dd, J = 8.2, 3.4 Hz, H-15), 3.20 (1H, m, H-3), 2.03 (1H, m, H-19b), 1.93 (1H, m, H-16b), 1.67 (2H, m, H-2b, H-7b), 1.64 (2H, m, H-2a, H-16a), 1.63 (2H, m, H-1b, H-11b), 1.62 (1H, m, H-6b), 1.53 (1H, m, H-6a), 1.49 (1H, m, H-11a), 1.46 (1H, m, H-18), 1.45 (1H, m, H-7a), 1.38 (1H, m, H-22b), 1.36 (1H, m, H-19a), 1.33 (1H, m, H-12b), 1.25 (2H, m, H-21), 1.10 (3H, s, H-27), 1.02 (1H, m, H-12a), 1.00 (1H, m, H-22a), 0.99 (2H, m, H-1a, H-9), 0.97 (3H, s, H-23), 0.95 (3H, s, H-29), 0.92 (3H, s, H-24), 0.91 (6H, s, H-26, H-30), 0.88 (1H, m, H-5), 0.82 (3H, s, H-28), 0.80 (3H, s, H-25); ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 158.3 (C-14), 117.1 (C-15), 79.3 (C-3), 55.7 (C-5), 49.5 (C-18), 48.9 (C-9), 41.5 (C-19), 39.2 (C-8), 39.0 (C-4), 38.2 (C-1), 37.9 (C-10, C-13, C-17), 36.9 (C-16), 36.0 (C-12), 35.3 (C-7), 33.9 (C-21), 33.5 (C-29), 33.3 (C-22), 30.1 (C-26), 30.0 (C-28), 29.0 (C-20), 28.2 (C-23), 27.3 (C-2), 26.1 (C-27), 21.5 (C-30), 19.0 (C-6), 17.7 (C-11), 15.7 (C-25), 15.6 (C-24).

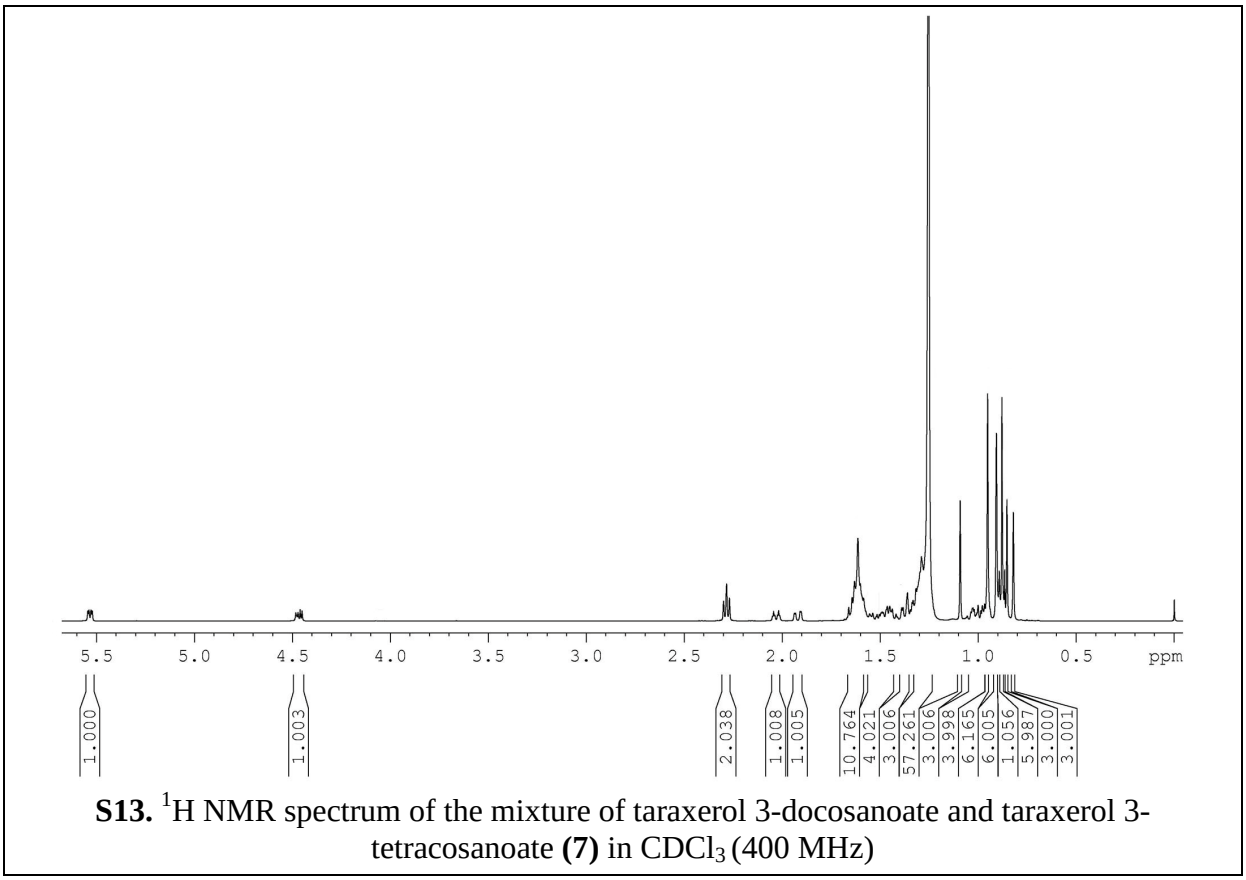


S11. ^{1}H NMR spectrum of taraxerol **(6)** in $CDCl_3$ (400 MHz)

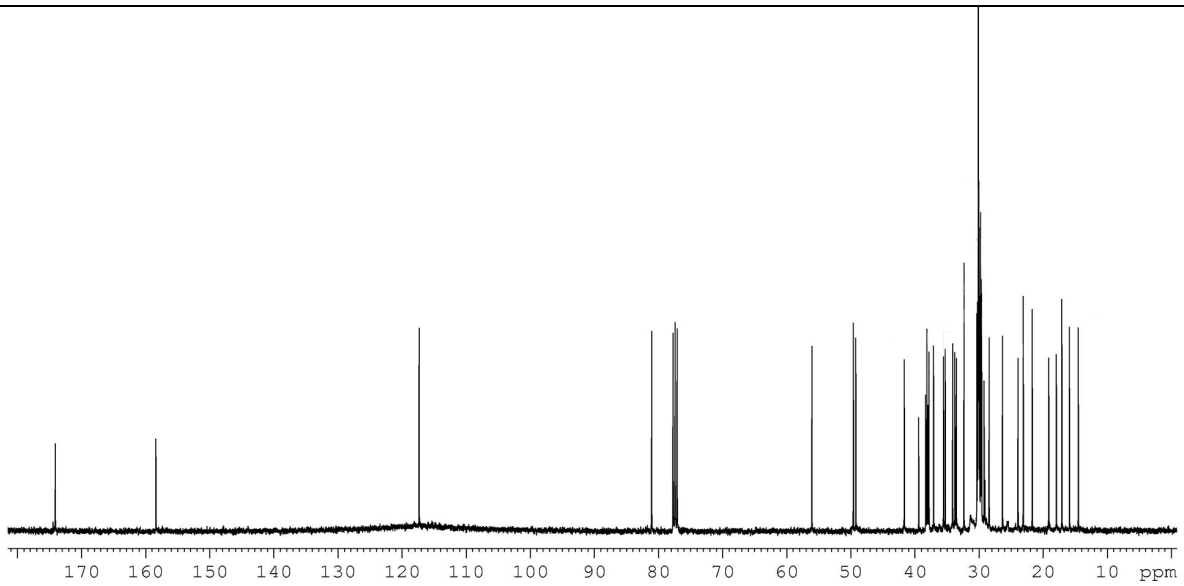


S12. ^{13}C NMR spectrum of taraxerol **(6)** in $CDCl_3$ (100 MHz)

A mixture of taraxerol 3-docosanoate (13α-methyl-27-norolean-14-en-3β-docosanoate) and taraxerol 3-tetracosanoate (13α-methyl-27-norolean-14-en-3β-tetracosanoate) **(7)**: white powder; mp 176-177°C; FABMS *m/z* (rel. int. %): 778 $[M+1]^+$ (1), 750 $[M+1]^+$ (3), 423 (3), 409 (36), 271 (17), 203 (22), 69 (96), 55 (100); EIMS *m/z* (rel. int. %): 425 (1), 409 (9), 393 (5), 369 (9), 284 (10), 269 (15), 218 (19), 204 (100), 189 (19), 57 (31); IR υ_{max} (KBr cm^{-1}): 2917, 2852, 1734, 1472, 1376, 1175, 1001, 716; ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 5.53 (1H, dd, *J* = 8.2, 3.1 Hz, H-15), 4.47 (1H, dd, *J* = 10.4, 5.6 Hz, H-3), 2.29 (2H, t, *J* = 7.4 Hz, CH_2COO), 2.03 (1H, m, H-19b), 1.92 (1H, m, H-16b), 1.66 (2H, m, H-2b, H-7b), 1.64 (2H, m, H-2a, H-16a), 1.63 (2H, m, H-1b, H-11b), 1.61 (1H, m, H-6b), 1.56 (1H, m, H-6a), 1.50 (1H, m, H-11a), 1.46 (1H, m, H-18), 1.45 (1H, m, H-7a), 1.39 (1H, m, H-12b), 1.36 (1H, m, H-22b), 1.29 (1H, m, H-19a), 1.26 (38H, m, H-21, $(CH_2)_{n-1}$, n = 20, 22), 1.10 (3H, s, H-27), 1.03 (2H, m, H-12a, H-22a), 1.00 (2H, m, H-1a, H-9), 0.95 (6H, s, H-23, H-29), 0.91 (6H, s, H-24, $C\underline{H}_3(CH_2)_{n-1}$, n = 20, 22), 0.88 (6H, s, H-26, H-30), 0.87 (1H, m, H-5), 0.86 (3H, s, H-28), 0.82 (3H, s, H-25); ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 174.0 (CO), 158.4 (C-14), 117.3 (C-15), 81.0 (C-3), 56.0 (C-5), 49.6 (C-18), 49.2 (C-9), 41.6 (C-19), 39.4 (C-4), 38.3 (C-8), 38.1 (C-1, C-17), 38.0 (C-13), 37.8 (C-10), 37.1 (C-16), 35.5 (C-12), 35.2 (C-7), 34.1 (C-21), 33.7 (C-29), 33.5 (C-22), 32.3 ($\underline{C}H_2COO$), 30.3 (C-26), 30.2 (C-28), 30.1-29.7 ($(CH_2)_{n-1}$, n = 20, 22), 29.6 (C-2), 29.2 (C-20), 28.4 (C-23), 26.3 (C-27), 21.7 (C-30), 19.1 (C-6), 17.9 (C-11), 17.0 (C-25), 15.9 (C-24), 14.5 ($\underline{C}H_3(CH_2)_{n-1}$, n = 20, 22). Capillary GC and GC-MS analysis of the products of *trans*-esterification of **(7)** indicated it was a mixture of taraxerol 3-docosanoate and taraxerol 3-tetracosanoate.



S13. ^{1}H NMR spectrum of the mixture of taraxerol 3-docosanoate and taraxerol 3-tetracosanoate **(7)** in $CDCl_3$ (400 MHz)

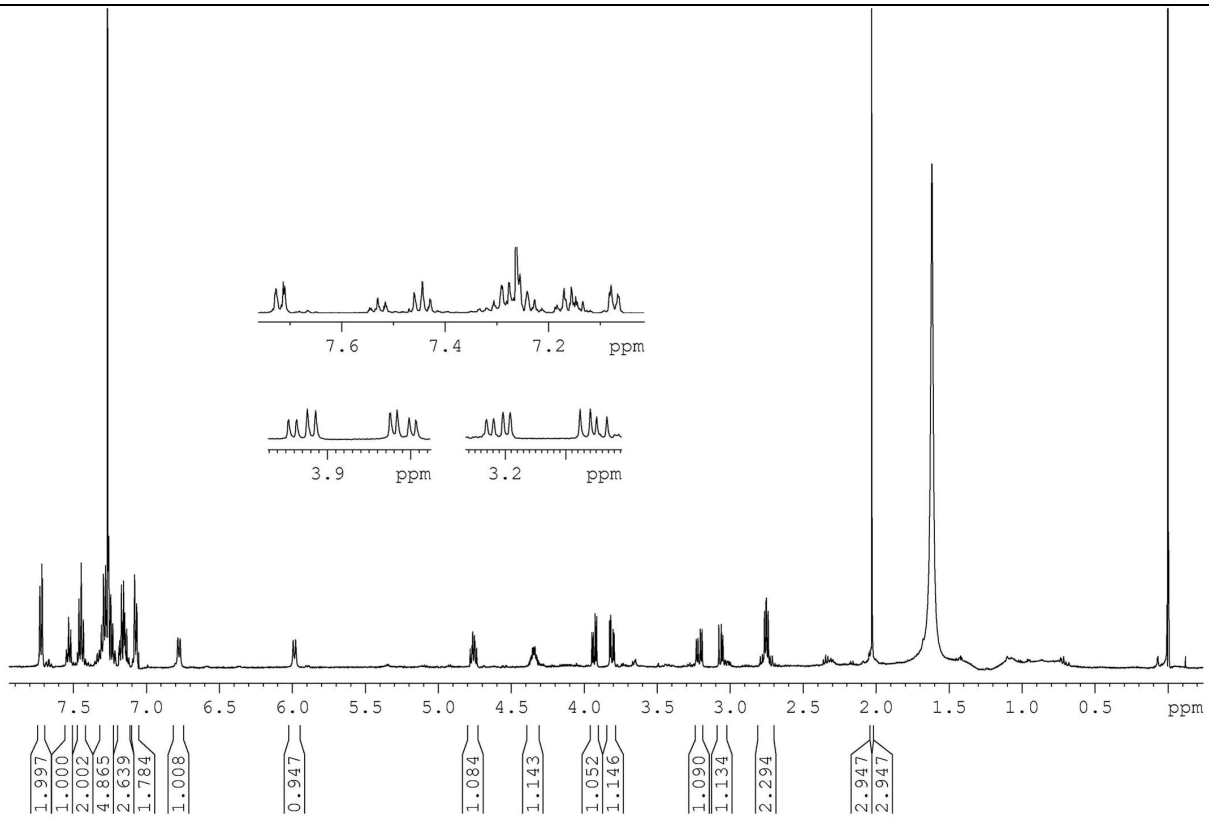


S14. ^{13}C NMR spectrum of the mixture of taraxerol 3-docosanoate and taraxerol 3-tetracosanoate **(7)** in $CDCl_3$ (100 MHz)

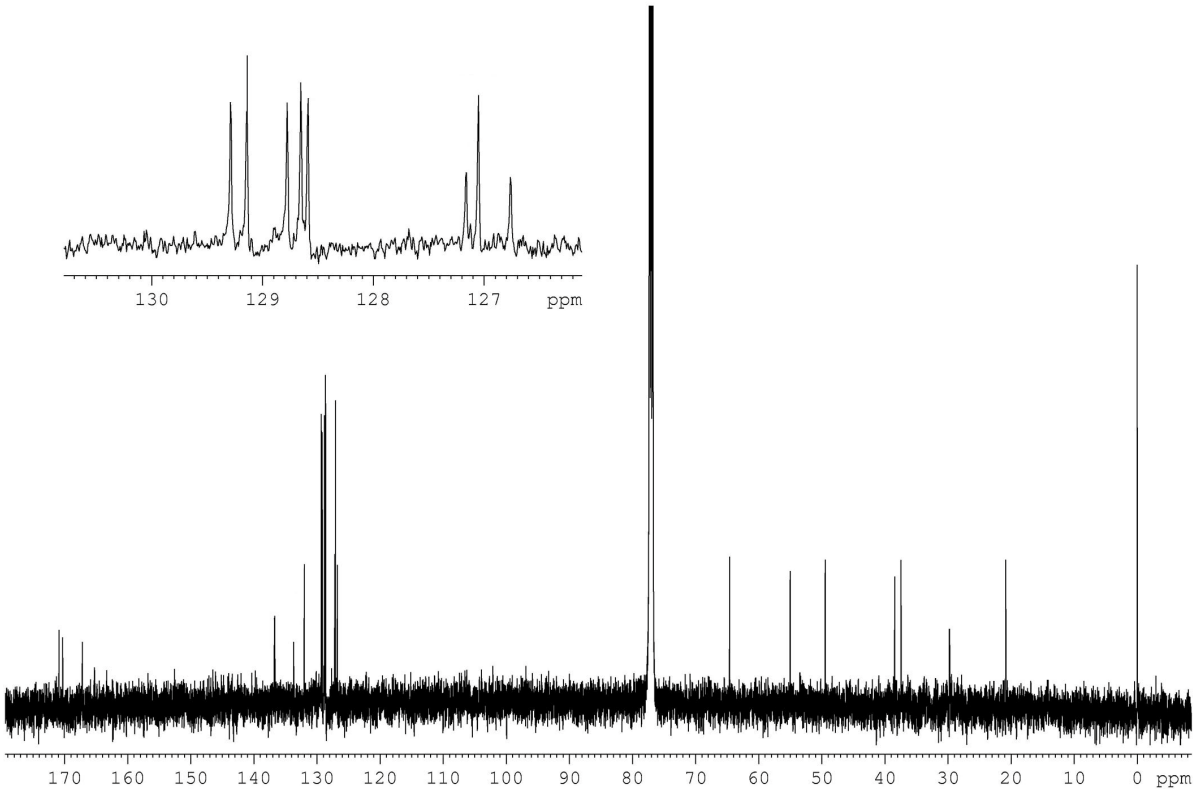
Table 2. GC analysis of *trans*-esterified products of **(7)**

Peak No	RT (min)	%	Compound
1	37.99	33.01	Methyl docosanoate
2	40.90	66.99	Methyl tetracosanoate

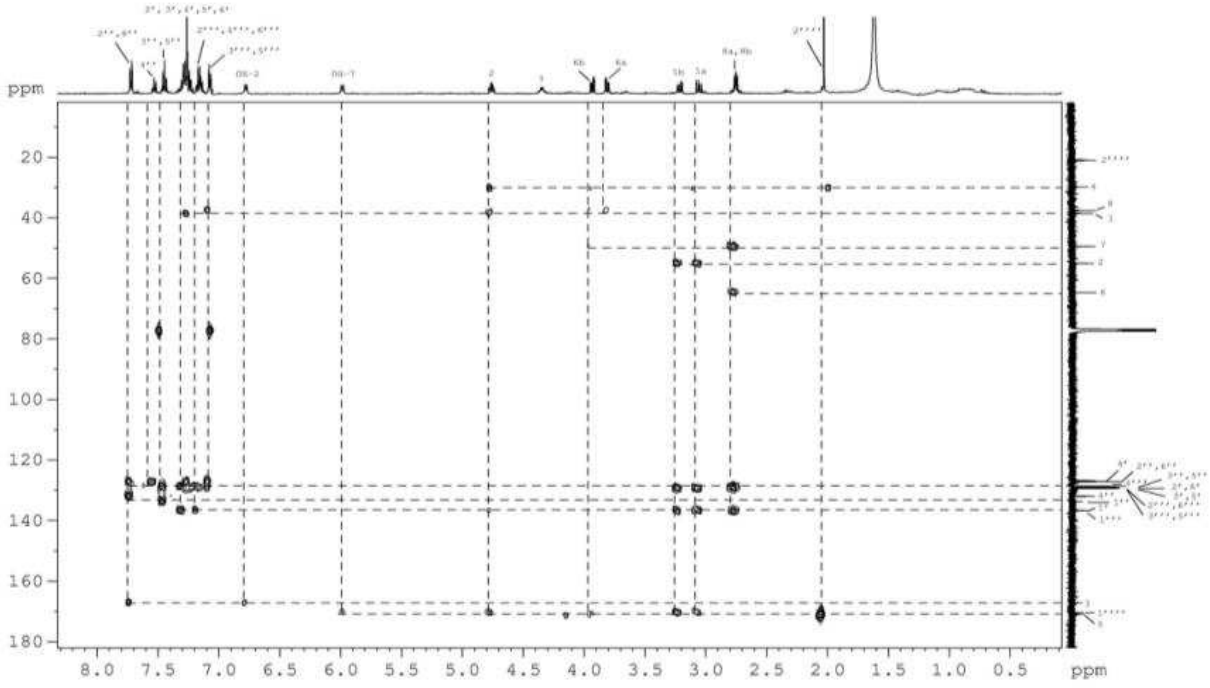
4-Acetyl-2, 7-dihydroxy-1, 4, 8-triphenyloctane-3, 5-dione **(8)**: white powder; mp 171-172°C; EIMS *m/z* (rel. int. %): 444 M^+ (2), 252 (44), 224 (39), 105 (100), 77 (25); IR υ_{max} (KBr cm^{-1}): 3445, 2919, 2846, 1720, 1625, 1382, 1105; ^{1}H NMR (500 MHz, $CDCl_3$): δ_H 7.72 (2H, d, *J* = 7.3 Hz, H-2'',H-6''), 7.53 (1H, t, *J* = 7.5 Hz, H-4''), 7.44 (2H, t, *J* = 7.9 Hz, H-3'', H-5''), 7.26 (5H, m, H-2', H-3', H-4', H-5' and H-6'), 7.16 (3H, m, H-2''', H-4''' and H-6'''), 7.09 (2H, d, *J* = 6.5 Hz, H-3''', H-5'''), 6.76 (1H, d, *J* = 7.5 Hz, OH-2), 5.96 (1H, d, *J* = 8.9 Hz, OH-7), 4.76 (1H, m, H-2), 4.35 (1H, m, H-7), 3.93 (1H, dd, *J* = 11.3, 4.8 Hz, H-6b), 3.81 (1H, dd, *J* = 11.3, 4.2 Hz, H-6a), 3.22 (1H, dd, *J* = 14.0, 5.8 Hz, H-1b), 3.05 (1H, dd, *J* = 14.0, 8.5 Hz, H-1a), 2.76 (2H, m, H-8a, H-8b), 2.05 (3H, s, H-2''''); ^{13}C NMR (125 MHz, $CDCl_3$): δ_C 170.8 (C-5), 170.2 (C-1''''), 167.1 (C-3), 136.7 (C-1'''), 136.6 (C-1'), 133.6 (C-1''), 131.9 (C-4''), 129.3 (C-3''',C-5'''), 129.1 (C-2''', C-6'''), 128.8 (C-3', C-5'), 128.7 (C-2', C-6'), 128.6 (C-3'', C-5''), 127.2 (C-4'''), 127.0 (C-2'', C-6''), 126.8 (C-4'), 64.6 (C-6), 55.0 (C-2), 49.4 (C-7), 38.4 (C-1), 37.4 (C-8), 29.7 (C-4), 20.8 (C-2'''').



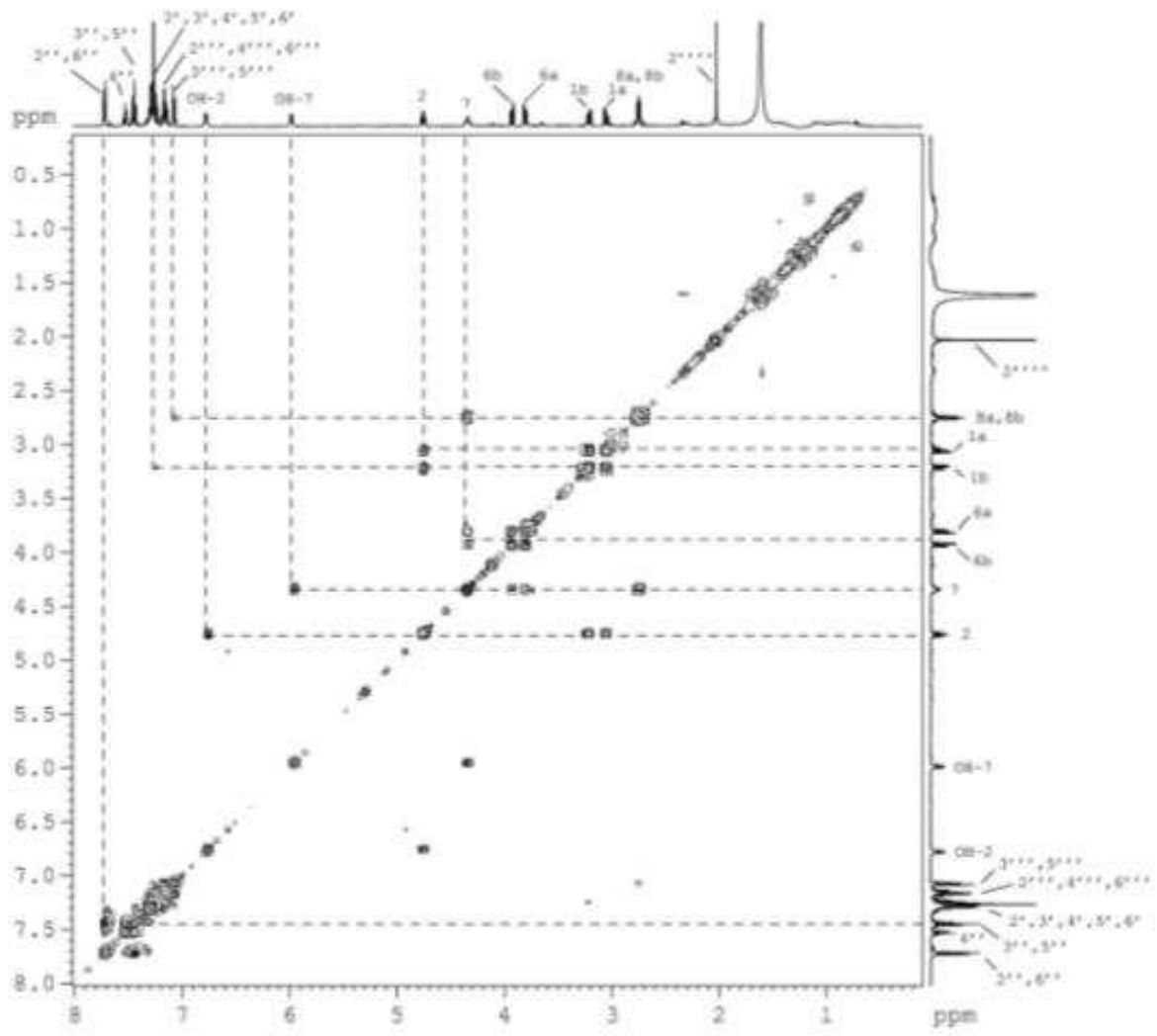
S15. ^{1}H NMR spectrum of 4-acetyl-2,7-dihydroxy-1,4,8-triphenyloctane-3,5-dione **(8)** in $CDCl_3$ (500 MHz)



S16. ^{13}C NMR spectrum of 4-acetyl-2,7-dihydroxy-1,4,8-triphenyloctane-3,5-dione **(8)** in $CDCl_3$ (125 MHz)

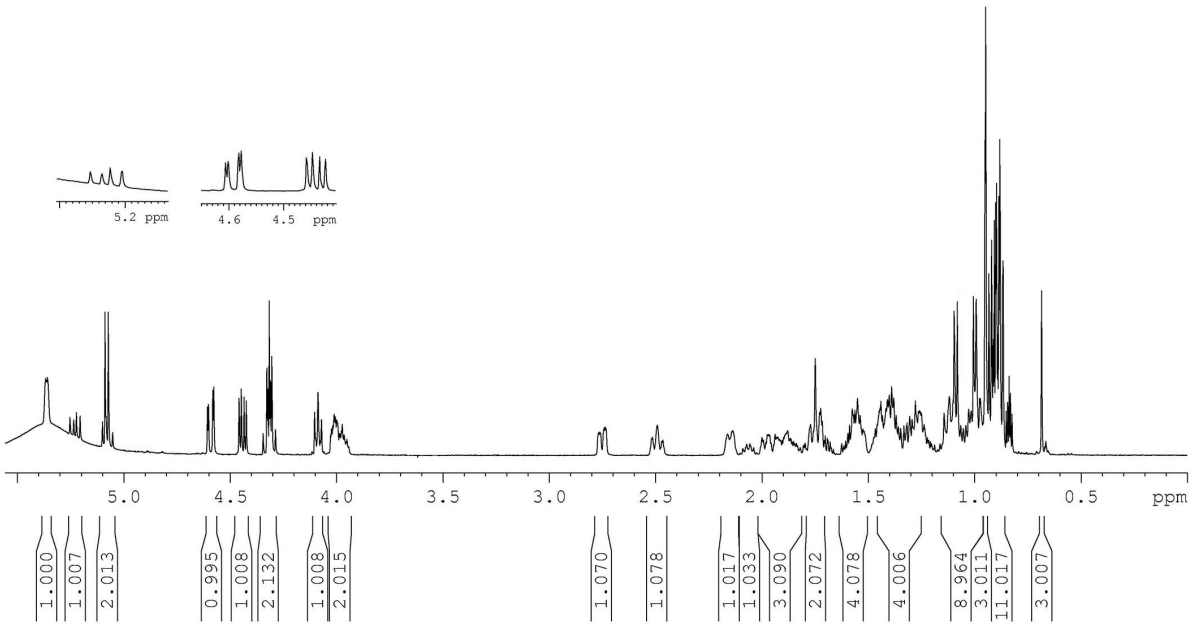


S17. HMBC spectrum of 4-acetyl-2,7-dihydroxy-1,4,8-triphenyloctane-3,5-dione **(8)** in $CDCl_3$ (500 MHz, $CDCl_3$)

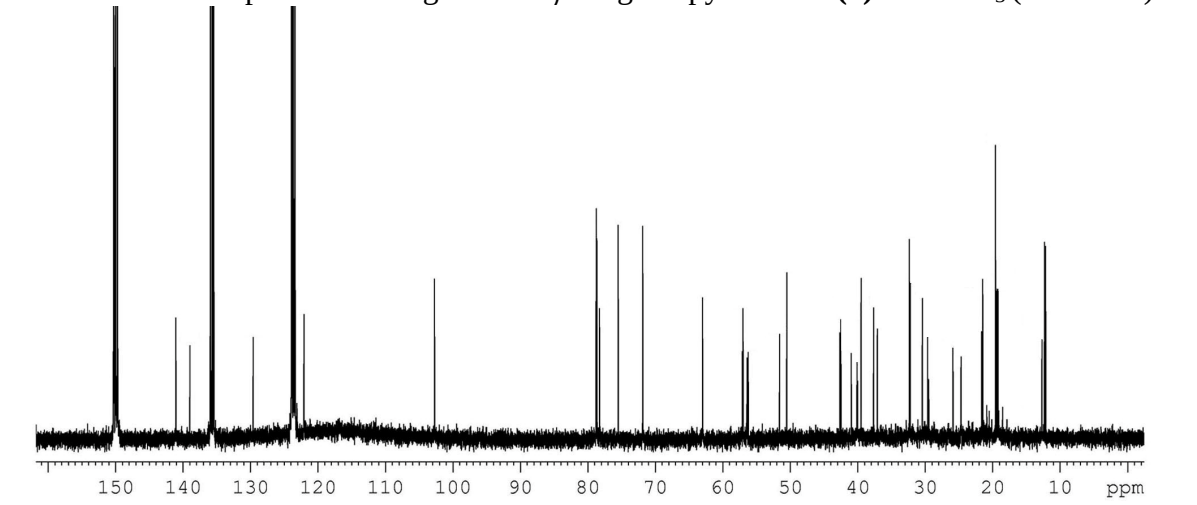


S18. ^{1}H-^{1}H COSY spectrum of 4-acetyl-2,7-dihydroxy-1,4,8-triphenyloctane-3,5-dione **(8)** in $CDCl_3$ (500 MHz, $CDCl_3$)

Stigmasterol 3-*O*-*β*-D-glucopyranoside [stigmast-5,22(*E*)-dien-3-*O*-*β*-D-glucopyranoside] **(9)**: white powder; mp 288-290°C; FABMS *m/z* (rel. int. %): 575 $[M+1]^+$ (5), 411 (10), 397 (67), 383 (18), 255 (13), 161 (32), 136 (42), 55 (100); IR υ_{max} (KBr cm^{-1}): 3413, 2934, 2868, 1634, 1463, 1368, 1167, 1071, 1024, 621; ^{1}H NMR (400 MHz, C_5D_5N): δ_H 5.35 (1H, m, H-6), 5.20 (1H, dd, *J* = 15.1, 8.6 Hz, H-22), 5.06 (2H, m, H-23, H-1'), 4.59 (1H, d, *J* = 11.8 Hz, H-6'b), 4.44 (1H, dd, *J* = 11.8, 5.4 Hz, H-6'a), 4.33 (2H, m, H-3', H-4'), 4.10 (1H, m, H-2'), 4.01 (1H, m, H-5'), 3.98 (1H, m, H-3), 2.75 (1H, d, *J* = 13.9 Hz, H-4b), 2.50 (1H, m, H-4a), 2.13 (1H, m, H-2b), 2.03 (1H, m, H-20), 1.97 (1H, m, H-12b), 1.87 (1H, m, H-7b), 1.83 (1H, m, H-16b), 1.73 (1H, m, H-2a), 1.71 (1H, m, H-1b), 1.57 (1H, m, H-24), 1.54 (2H, m, H-7a, H-25), 1.53 (1H, m, H-15b), 1.42 (2H, m, H-11a, H-11b), 1.37 (1H, m, H-8), 1.26 (1H, m, H-16a), 1.10 (1H, m, H-12a), 1.08 (1H, m, H-17), 1.03 (1H, m, H-1a), 1.01 (1H, m, H-15a), 0.97 (3H, s, H-19), 0.95 (2H, m, H-28), 0.92 (3H, br s, H-21), 0.91 (1H, m, H-14), 0.89 (1H, br s, H-9), 0.87 (3H, d, *J* = 6.6 Hz, H-26), 0.85 (3H, br s, H-29), 0.83 (3H, br s, H-27), 0.66 (3H, s, H-18); ^{13}C NMR (100 MHz, C_5D_5N): δ_C 141.1 (C-5), 139.0 (C-22), 129.6 (C-23), 122.1 (C-6), 102.8 (C-1'), 78.8 (C-3'), 78.7 (C-5'), 78.3 (C-3), 75.5 (C-2'), 71.9 (C-4'), 63.0 (C-6'), 57.0 (C-14), 56.4 (C-17), 51.6 (C-24), 50.5 (C-9), 42.6 (C-13), 41.0 (C-20), 40.1 (C-12), 39.5 (C-4), 37.7 (C-1), 37.1 (C-10), 32.4 (C-7), 32.2 (C-8, C-25), 30.4 (C-2), 29.6 (C-16), 25.9 (C-28), 24.7 (C-15), 21.7 (C-21), 21.5 (C-11, C-26), 19.6 (C-19), 19.4 (C-27), 12.7 (C-29), 12.3 (C-18).



S19. ^{1}H NMR spectrum of stigmasterol *β*-D-glucopyranoside **(9)** in $CDCl_3$ (400 MHz)



S20. ^{13}C NMR spectrum of stigmasterol *β*-D-glucopyranoside **(9)** in $CDCl_3$ (100 MHz)

Micro-dilution antibacterial assay: Two mL cultures of two Gram-positive bacteria, namely *Bacillus subtilis* (ATCC6633) and *Staphylococcus aureus* (ATCC12600), and three Gram-negative bacteria, namely *Escherichia coli* (ATCC25922), *Klebsiella pneumoniae (*ATCC13883) and *Salmonella typhimurium* (ATCC14028) were prepared and placed in an incubator overnight at 37°C. The overnight-cultures were diluted with sterile nutrient broth (Merck) (500 µL bacteria / 50 mL broth) to yield density of bacterial cells between 10^5-10^6 cell/mL. The investigated samples were re-suspended to a concentration of 4 mg/mL with ethanol to yield a final concentration of 1 mg/mL in the assay for the first well. For each of the five bacteria used, 100 µL of the tested samples were two-fold serially diluted with 100 µL sterile distilled water in a sterile 96-well micro-plate. A similar two-fold serial dilution of gentamicin sulfate (1 mg/mL) was used as a positive control against each bacterium. One hundred µL of each bacterial culture were added to each well of the tested samples, gentamicin sulfate (positive control), ethanol, water and the nutrient broth (negative controls). The plates were covered and incubated overnight at 37°C. To indicate bacterial growth, 50 µL of 0.2 mg/mL *p*-iodonitrotetrazolium violet (INT, Sigma) was added to each well and the plates incubated at 37°C for 30 min. Bacterial growth in the wells was indicated by a red colour, whereas clear wells indicated inhibition by the tested substances. This assay was repeated three times.

***Acetylcholinesterase enzyme inhibitory activity*:** Hydrolysis of acetylthiocholine was monitored by the formation of yellow 5-thio-2-nitrobenzoate anion resulting from the reaction of thiocholine with dithiobisnitrobenzoate ion. Acetylthiocholine iodide (ATCl), acetylcholinesterase (AChE) from electric eels (type VI-S lypophilised powder), 5,5-dithiobis-2-nitrobenzoic acid (DTNB) and galanthamine were obtained from Sigma-Aldrich. The following buffers were used; buffer A: 50 mM Tris-HCl, pH 8; buffer B: 50 mM Tris-HCl, pH 8 containing 0.1% bovine serum albumin (BSA); buffer C: 50 mM Tris-HCl, pH 8, containing 0.1 M NaCl and 0.02 M $MgCl_2.6H_2O$. The assay was performed using an Opsys MR 96-well microplate reader. 25 µL of 15 mM ATCl in water, 125 µL of 3 mM DTNB in buffer C, 50 µL of buffer B and 25 µL of a serially diluted (two-fold) solution of the crude extracts and the isolated compounds (final concentration of 100 µg/mL) were added in the 96-well plates. The absorbance was measured every 45 s (three times) at 405 nm (background). Then, 25 µL of 0.2 U/mL solution of enzyme was added. The absorbance was again measured every 45 s (eight times). Serially diluted galanthamine (25 µL) was used as a positive control (5 µg/mL) and 10% methanol in buffer A (25 µL) was used as a blank (negative control). The rate of reaction was calculated. Any increase in absorbance due to the spontaneous hydrolysis of the substrate was corrected by subtracting the ratio of reaction before adding the enzyme from the rate after adding the enzyme. Percentage inhibition was calculated by comparing the reaction rates of the sample to the blank (10% methanol in buffer A). The IC_{50} values were calculated by plotting a concentration response curve (100, 50 &25 µg/mL).