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NEW DITERPENES FROM A NEW SPECIES OF LOBOPHYTUM SOFT CORAL OF THE SOUTH ANDAMAN COAST

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ABSTRACT : Two new cembrenoid diterpenes (10) and (13) and one novel neodolabellane diterpene (16) have been isolated from a new species of Lobopytum soft coral of the South Andaman Coast, along with the known diterpenes (2) and (3) and lipids (1), (4), (5), (6), (7), (8) and (9). The structures were determined from spectral data and chemical conversions.

Soft corals contain a variety of bioactive compounds[1]. Andaman and Nicobar Islands in the Bay of Bengal abound in soft corals. In this communication we report the isolation and the structure determination of several secondary metabolites, including three new diterpenes from a new species of **Lobophytum** soft coral collected from the South Andaman Coast.

The soft coral (2.50 kg. dry weight) was collected manually from the South Andaman Coast in the Bay of Bengal, India in March 1989. This coral has been identified as a new species of **Lobophytum** by **Dr. Phil Alderslade**, Northern Territory Museum of Arts and Science, Australia. A specimen of this coral registered as NTMC 10798 was deposited at NTM. Column chromatography on SiO_2 of the EtOAc soluble material from the methanol extract of the coral gave hexadecanoic acid hexadecylester[2] (1), 1E, 3E, 7E, 11:12-epoxy-1,3,7-cembratriene[3] (2), 3S, 4S, 11S, 12S, 1E, 7E-3:4, 11:12-bisepoxy-1,7-cembradiene[4] (3), 1-O-hexadecyl-2,3-dihexadecanoyl glycerol[5,6] (4); a mixture of dihydrobrassicasterol[7,8] (5) and gorgosterol[9] (6); 1-O-hexadecyl-3-

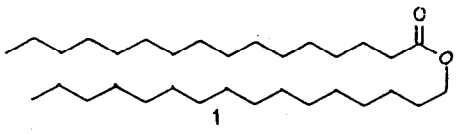
hexadecanoyl glycerol (7); a 1:1 mixture of 1-O-hexadecyl glycerol[5] (8) (chimyl alcohol) and 1-O-octadecyl glycerol[5] (9) (batyl alcohol) in addition to three new diterpenes designated as LN01, 02 and 03. The structures of the known compounds were determined by comparison of their physical and spectral data with the published data.

LN01, colourless oil, $(\alpha)_D^{30}$ -15°, $\nu_{max}^{CHCl_3}$ 1735, 1655 and 850 cm^{-1}, $C_{22}H_{36}O_2$, did not show the M^+ ion in the EI^+ spectrum but showed the (M+1) ion at m/z 333 in the CI^+ spectrum. In both the spectra there was a prominent ion (in the latter it was the base peak) at m/z 289.2566, corresponding to $C_{20}H_{33}O$ ($M-COCH_3$) and another prominent ion at m/z 271 (M-61). Thus, the two oxygens in LN01 were present in the form of an acetate.

The ^1H NMR spectrum of LN01 was very similar to that of (2), indicating their close relationship. The ^1H NMR spectrum of LN01 (90 MHz) showed the C-2, C-3 protons (δ5.80s), the C-7 H (5.22m), the C-18 and C-19 methyls δ1.65s (3H), 1.55s (3H), and the isopropyl group (C-16, C-17 methyls): δ1.10d, J=7.0, (6H), as in (2). The C-11 proton (δ2.88t) and the C-20 methyl, (δ1.26s) signals were missing but in their place signals due to a secondary methyl δ 0.98d, J=7.0 (3H) an acetate δ 2.03s (3H) ($OCOCH_3$) and a multiplet at δ4.90 (1H) ($-CH-OCOCH_3$) appeared. Thus LN01 and (2) differed only at the C-11, C-12 positions, the former having a C-11 acetoxy and secondary methyl at C-12 and the latter having the C-11, C-12 epoxide. Thus LN01 was IE, 3E, 7E -11-acetoxy-1,3,7-cembratriene (10), a new cembrenoid diterpene. Reduction of LN01 with LAH in either gave the alcohol[3] (11) which was obtained also by a similar reduction of (2) (identified by Co-TLC), thus confirming the assigned structure (**10**) for LN01.

LN02, gum $(\alpha)_D^{30}$ +1.72°, showed an ion at m/z 318 (M^+) and a prominent ion at m/z 317 (M-1): found m/z 317.2120, calc. for $C_{20}H_{29}O_3$: 317.2118. Thus the molecular formula of LN02 was $C_{20}H_{30}O_3$, with six degrees of unsaturation. The IR spectrum of LN02 did not show hydroxyl or carbonyl groups. The ^1H NMR spectrum of LN02 showed signals due to three olefinic protons: δ 5.43 brd, J=9.60 (1H), H-7; 5.02m (1H), H-13; 4.90m, (1H), H-6; two oxygen bearing methine protons, δ 4.90m (1H), H-11 and 3.04t, (1H), H-3, and five methyls; δ 1.83s (6H), 1.64s (3H), 1.27s (3H), 1.26s (3H). The presence of five methyls indicated the cembrenoid nature of LN02. Since the isopropyl group and one methyl group were involved in double bonds and since there were only three olefinic protons, LN02 must contain a disubstituted double bond also. Thus LN02 was a cembrenoid with one di, one tri and one tetrasubstituted double bond.

LN02 contained three oxygens. Since there was no carbonyl or OH groups in the molecule, the three oxygens must be involved in ether linkages. The chemical shifts of the two methyl groups (δ1.27s, 1.26s) in LN02 showed that they were bonded to



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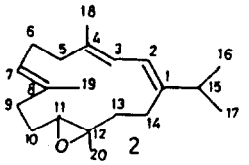

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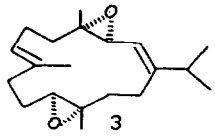

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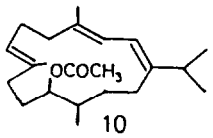

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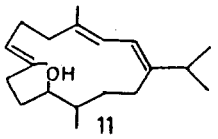

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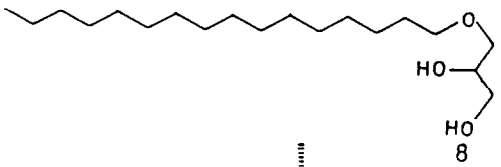

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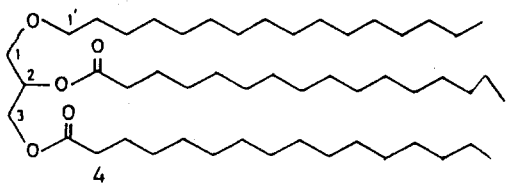

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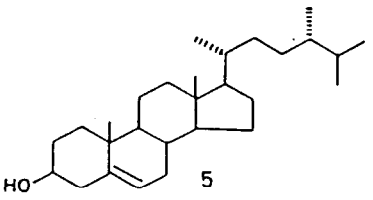

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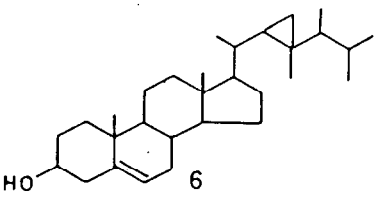

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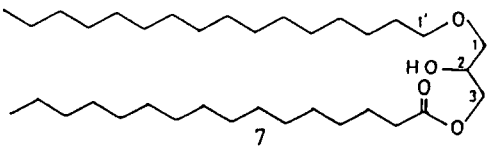

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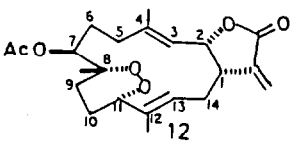

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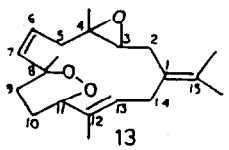

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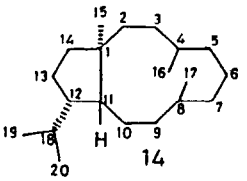

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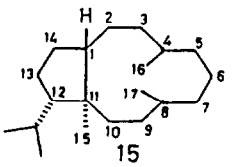

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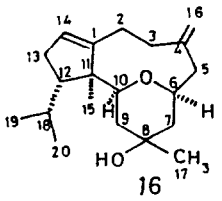

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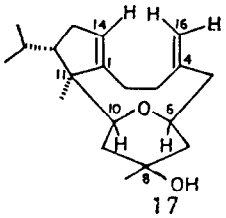

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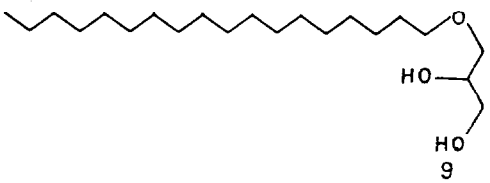

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oxygen bearing carbons, thus indicating their connection with the three oxygens in the molecule. Two epoxy rings involving these two methyl bearing carbons would account for only two oxygens. All the three oxygens could be accounted for, however, by one cyclic peroxide and one epoxide. LN02 gave a positive KI test for peroxides. Thus LN02 was a new cembrenoid diterpene.

The H-11 proton at δ4.90m in LN02 was deshielded for a proton bonded only to an epoxy carbon or a peroxy carbon. In the naturally occurring cembrenoid peroxide, denticulatolide (12), isolated from the soft coral **Lobophytum denticulatum**[10], H-11, the α-peroxy proton flanked by the Δ^{12} double bond showed a multiplet at δ4.35. Therefore in LN02 also the less substituted end of the peroxide and the trisubstituted double bond were adjacent to each other. H-11 would be deshielded less if it was flanked by the epoxide in LN02. Since the isopropyl group was involved in the tetrasubstituted double bond, the position of the latter was $\Delta^{1(15)}$ in LN02.

LN02 did not show conjugation. Thus a Δ^{2} or Δ^{13} position for the disubstituted double bond was excluded. There are two possibilities for a stable six membered cyclic peroxide to be located in the $\Delta^{1(15)}$ cembrane ring involving any one of the three methyl groups: (a) the C_4-C_7 peroxide (identical with the C_9-C_{12} peroxide) and (b) C_5-C_8 peroxide (identical with the C_8-C_{11} peroxide). The former possibility (a), however, could be excluded for LN02 because in such a system the unconjugated double bond could not be accommodated. Thus LN02 had the C_8-C_{11} peroxide and, consequently, the Δ^{12} trisubstituted double bond.

Since the epoxide was associated with the remaining methyl group, the epoxide could be at C_3-C_4 or C_4-C_5. As the protons of the disubstituted double bond were not deshielded (as would have been the case if they were located at C_9-C_{10}, enclosed by the peroxy group), the double bond could not be at Δ^{9}. It could not be at Δ^{2} either because it would be conjugated. Thus the double bond could be located at Δ^{5} or Δ^{6}. If the epoxide was at C_4-C_5, the double bond would be at Δ^{6} in which case the C_5 epoxy proton should appear as a doublet. The NMR spectrum of LN02 showed the H-3 at δ3.04 as a triplet. Thus, irrespective of the position of the disubstituted double bond, the epoxide could be located only at C_3-C_4 in LN02.

There were only two positions for the disubstituted double bond in LN02. These were Δ^{5} and Δ^{6}. With the available evidence a choice cannot be made between these two positions. However, by analogy with other naturally occurring cembrenoids, the Δ^{6} double bond seems to be more likely. An isolated Δ^{6} double bond or a precursor to form a Δ^{6} double bond could be found in many naturally occurring cembrenoids, e.g. denticulatolide (12), alcynol B[11], and the mayols[12]. The disubstituted double bond in LN02 was tentatively assigned the Δ^{6} position. The IR spectrum of LN02 did

not show any band at 960 cm^{-1}, so the Δ^6 double bond was cis. From the above evidence, LN02 was 1(15), 6Z, 12E -3,4-epoxy-8, 11-peroxy-1(15), 6,12-cembratriene (13), a new cembrenoid peroxide.

LN03, gum, $(\alpha)_D^{30}$-66.7°, $C_{20}H_{32}O_2$, mass spectrum (CI^+): m/z 322 ($M+\dot{N}H_4$) (40%) 305 (M+1) (20), 287(M-OH) (100), 269 (60); found m/z 269.2314 corresponding to $C_{20}H_{29}$; m/z 269.2271. The ^{13}C NMR spectrum of LN03 showed 20 carbons as, a trisubstituted double bond and an end methylene group (δ149.91s, 147.37s, 122.71d, 111.66t), one tertiary hydroxyl bearing carbon, (δ81.40s), one disubstituted ether (δ62.23d, 54.34d), six methylene carbons (δ40.58t, 36.97t, 28.18t, 26.35t, 25.98t, 24.32t), two methine carbons (δ51.55d, 30.59d), one quaternary carbon, (δ62.23s) and four methyl groups (δ23.88q, 23.79q, 20.97q, 20.61q). The ^1H NMR spectrum of LN03 showed the proton on the trisubstituted double bond at δ4.96m and the end methylene protons at δ4.90s (1H) and δ4.69s (1H). It showed two protons geminal to an oxygen function at δ2.85m (2H), the two secondary methyls of the isopropyl group at δ1.09d, J=6.70 (3H) and δ1.03d, J=6.80 (3H) and two tertiary methyls at δ1.11s (3H) and δ1.08s (3H). The molecular formula of LN03 indicates five degrees of unsaturation in the molecule. Since the compound had two double bonds and one cyclic ether linkage, the two remaining two degrees of unsaturation must be due to a carbobicyclic structure in the molecule.

The ^1H and ^{13}C NMR spectra of LN03 were most helpful in fixing the carbon framework and fixing the functional groups in the molecule. From the chemical shifts and the multiplicities of the carbons (one quaternary sp^3 carbon; δ62.23s; two methine carbons, δ51.55d, 30.59d, six methylene carbons, δ40.58t, 36.97t, 28.18t, 26.35t, 25.98t, 24.32t), four methyls and an end methylene in the ^{13}C NMR spectrum of LN03, the bicyclic carbon framework in the molecule could only be either the dolabellane (14) or the neodolabellane (15) system. Dolabellane (14) and neodobellane (15) systems differ only at the C-1 and C-11 positions, the former having the C-1 methyl and the latter having the C-11 methyl.

The chemical shift of the trisubstituted double bond proton, δ4.96m, in LN03, was shielded for a proton of a normal trisubstituted double bond (about δ5.50 observed in related systems). Thus LN03 had a group located in a position to influence the trisubstituted double bond. Since there were no methyls on a double bond, the trisubstituted double bond in LN03 could be at Δ^{10} or Δ^{12} (dolabellane system) or at Δ^1 or $\Delta^{1(14)}$ (neodolabellane system) and the end methylene group at C-4 or C-8 (since LN03 showed only four methyls, the end methylene group must replace the fifth methyl group). There are only two groups in LN03 which could influence the chemical shift of the trisubstituted double bond, the end methylene group and the ether linkage. Of these two, the end methylene group could influence the chemical

shift to a greater extent than the ether linkage. Thus the location of the end methylene group would fix the position of the trisubstituted double bond in LN03.

An examination of the molecular models of the dolabellane (14) and the neodolabellane (15) systems showed that with the end methylene group at C-4 and the trisubstituted double bond at $\Delta^{1(14)}$ [possible only with the neodobellane system (15)], H-14 could be shielded. In this position, it would be possible for the molecule to assume a conformation which would bring the C-4 end methylene ($\Delta^{4(16)}$ double bond) and the $\Delta^{1(14)}$ double bond very close and facing each other. This situation would not be possible in a dolabellane (14) system or even in the neodolabellane system with the end methylene group at C-8. This situation was possible only with the $\Delta^{1(14)}$ and $\Delta^{4(16)}$ dienes in a neodolabellane (15) system. Thus, the Δ^{10} or Δ^{12} (dolabellane system) or the Δ^{1} (neodolabellane system) for the trisubstituted double bond in LN03 were eliminated. Therefore, the observed shielding of H-14 fixes the neodolabellane (15) system for LN03 and the $\Delta^{1(14)}$ and $\Delta^{4(16)}$ positions for the two double bonds . Consequently, the remaining methyl and the hydroxyl groups were placed at C-8. The stereochemistry at C-8 in LN03, could not be fixed with the available evidence.

The two protons geminal to an oxygen function in LN03 appeared at δ 2.85m, suggesting that the disubstituted cyclic ether linkage did not have an allylic double bond or an α-oxygen carrying carbon at either end. This is possible only with a C_6-C_{10} ether bridge. Further, with a β cis-C_6-C_{10} ether bridge the $\Delta^{1(14)}$ and $\Delta^{4(16)}$ double bonds would come very close, facing each other, and the C-6 and C-10 hydrogens would become α-axial, thus experiencing shielding of H-14, H-6 and H-10 as had been observed in LN03. Thus the structure of LN03 could be represented by (16), a new diterpene belonging to the small group of neodolabellane diterpenoids[13,14,15].

The C_6-C_{10} ether bridge also explains the observed deshielding of the C-11 carbon and the shielding of the C-6, C-10 carbons in the ^{13}C NMR spectrum of LN03 (16). The C-11 carbon in the naturally occurring neodolabellanes[13,14,15] which do not have a substituted C-10 show a chemical shift around δ 50.0. However, with the C-10 substituted in LN03 the C-11 carbon is now surrounded by one more α-substituted carbon and thus can experience deshielding as has been observed (δ62.23s). Since the C-6 oxygen bearing carbon is surrounded on either side by a methylene group it should have the chemical shift of a normal alkyl ether at around δ60.0 (observed δ62.23d). The C-10 carbon is surrounded by a quaternary carbon on one side and by a methylene group on the other side and therefore should have chemical shift around δ55.0, as expected for the less substituted end of a trisubstituted ether bridge (observed δ 54.31d). A possible confirmation of LN03 (16) which would explain the observed data is shown in (17).

This new **Lobophytum** species contained large quantities of lipids and these lipids were present in practically all polarity ranges. Isolation of lipid free diterpenes was extremely difficult and involved repeated chromatography. The yields quoted above are isolated yields and are considerably lower than the actual amounts in the coral.

Experimental

IR spectra were recorded on a Shimadzu IR-308 double beam spectrometer and NMR spectra were taken in $CDCl_3$ with TMS as internal standard. Unless otherwise stated the ^1H NMR were taken at 250 MHz and the ^{13}C NMR at 62.9 MHz. Coupling constants are given in hertz (Hz). The CI^+ mass spectra were ammonia spectra.

Collection and Isolation

The soft coral (2.50 kg, after isolation) was collected manually from the South Andaman Coast in the Bay of Bengal, India in March 1989 and was immersed immediately in methanol (10L). The methanol extract was concentrated under reduced pressure to give a dark residue. This dark residue was extracted repeatedly with EtOAc. Removal of EtOAc from this extract gave a dark coloured gum (110g) which was chromatographed on SiO_2 (ACME, 100-200 mesh, 700gm in 80mm x 1m column) using solvent mixtures of increasing polarity from n-hexane (b.p. 66°) through EtOAc. Repeated chromatography of some of the resulting fractions gave compounds 1-16 in the order given below.

Hexadecanoic acid hexadecyl ester (1)

Silky solid, (9g) m.p. 50° (Lit.[2] m.p. 53-4°).

1E,3E,7E, 11:12 -Epoxy-1,3,7-cembratriene (2)

Colourless oil, (0.2g) $(\alpha)_D^{30}$ 115° (C,1.0 $CHCl_3$), (Lit.[3] $(\alpha)_D^{30}$ +117°). Found, m/z 288.2411 calc. for $C_{20}H_{30}O$ 288.2455. ^1H NMR: δ 5.89 ABq J=10.5 (2H) (the same signal was observed as a singlet in the 90 MHz spectrum), 5.23t, J=5.70 (1H), 2.80t, J=6.90 (1H), 1.72s (3H), 1.60s (3H), 1.26s (3H), 1.03d, J=6.80 (6H); ^{13}C NMR: δ 147.01s, 135.89s, 133.36s, 127.11d, 120.89d, 118.42d, 61.05s, 60.40d, 38.40t, 36.94t, 36.82t, 34.11d, 25.29t, 24.50t, 24.32t, 22.92q, 22.24q, 18.07q, 17.41q, 14.97q.

3S, 4S, 11S, 12S, 1E, 7E-3,4: 11,12-Bisepoxy cembra-1, 7-diene (3)

Colourless prisms (0.3g), m.p. 110°, $(\alpha)_D^{30}$ +50° (C,1.0, $CHCl_3$), (Lit.[4] m.p 109-10° $(\alpha)_D^{30}$ +53.5°). Found: m/z 304 (M^+) and m/z 287.2374 (M-OH): calc. for $C_{20}H_{31}O$, m/z 287.2376. ^1H NMR: δ 5.30t, (1H), 4.97d, J=6.50 (1H) 3.30d, J=6.60 (1H), 2.67m

(1H), 1.64s (3H), 1.29s (3H), 1.23s (3H), 1.03d, J=6.80 (6H). (Irradiation of the 4.97d made the 3.30d into a singlet), ^{13}C NMR: δ151.24s, 134.56s, 126.38d, 119.54d, 62.08d, 61.52s, 61.28s, 59.52d, 39.11t, 37.39t, 36.70t, 34.11d, 27.61t, 24.59t, 22.39q, 22.24t, 21.84q, 18.17q, 16.27q, 14.82q.

LN01, (1E, 3E, 7E-11-Acetoxy-1,3,7-cembratriene (10)

Colourless oil, (0.04g), $(\alpha)_D^{30}$-15° (C,0.5 $CHCl_3$), λ_{max}^{EtOH} 250nm (log ε 4.34). For IR and ^1H NMR data see Text. Compound (10) was stable when present in the mixture but decomposed slowly after purification. ^{13}C NMR values of (10) (after deducting the spectrum of the aliphatic component of the mixture of (10) and an aliphatic ether component) are δ174.15, 150.37, 140.65, 133.33, 129.03, 127.18, 122.80, 74.49, 37.43, 34.52, 31.91, 30.88, 26.47, 24.08, 23.99, 23.91, 21.11, 20.66, 18.34, 17.50, 16.47, 14.71.

LAH reduction of (10) to give the alcohol (11)

Compound (10) (10mg) in 5ml of dry ether was treated with 50mg of LAH. After refluxing the mixture for 2 hours, and workup of the reaction mixture gave the alcohol[3] (11) as a colourless oil (3mg), which was found to be identical (Co-TLC and ^1H NMR) with the product obtained by the reduction of (2) (10mg) (in 5ml dry ether) with LAH (20mg) for 2 hours.

1-O-Hexadecyl-2,3-dihexadecanoyl glycerol (4)

Colourless prisms (0.70g) m.p. 60-61°, $(\alpha)_D^{30}$+7.5°(C,1.0, $CHCl_3$), had the molecular formula of $C_{51}H_{100}O_5$, found m/z 537.5241 (M-$C_{16}H_{31}O_2$) calc. for $C_{35}H_{69}O_3$: 537.5250. $\nu_{max}^{CHCl_3}$ 1710cm^{-1}. Details of physical and spectral data for this compound were not reported previously. ^1H NMR : δ5.20m (1H), H-2; 4.34dd, J=11.90, 3.70 (1H), H-3; 4.16dd, J-11.90, 6.40 (1H), H-3; 3.54d, J=5.30 (2H), H-1; 3.43m (2H), H-1'; 2.31m (4H) 1.61m (6H), 1.26s (74H), 0.88t (9H); ^{13}C NMR : δ173.38s, 173.09s, 71.76t, 70.11d, 68.98t, 62.78t, 34.37t, 34.15t, 31.94t, 29.70t, 29.49t, 29.35t, 29.30t, 29.14t, 26.06t, 24.99t, 24.93t, 22.68t, 14.09q.

Compound (4) (100 mg) was refluxed with 5ml of 10% methanolic KOH for 4 hours. Workup gave 20 mg of 1-O-hexadecyl glycerol[5] (8), m.p. 62° and 54 mg of hexadecanoic acid, m.p. 60°.

Steroid mixture of (5) and (6)

The steroid mixture crystallized as colourless needles from methanol, (4g), m.p. 143-44°. It gave a positive LB test for a steroid and readily gave an acetate (Ac_2O-Py, RT., 2 hours), m.p. 153.55°. Both the alcohol and its acetate showed single spots on TLC (on normal as well as $AgNO_3$-impregnated SiO_2 plates) but their ^1H, ^{13}C NMR and mass spectral data indicated them to be mixtures consisting predominently of

dihydrobrassicasterol (5) and gorgosterol (6). This steroid mixture was not examined further.

1-O-Hexadecyl-3-hexadecanoyl glycerol (7)

Colourless prisms from methanol (0.06g) m.p. 58-60° $(\alpha)_D^{30}$+7.14° (C,0.35 $CHCl_3$). $\nu_{max}^{CHCl_3}$ 1730 cm^{-1}, $C_{35}H_{70}O_4$, did not show the molecular ion but showed ions at m/z 299 ($M-C_{16}H_{31}O_2$), ^1H NMR: δ4.15t (2H), H-3; 3.99m, (1H), H-2; 3.46m (4H), H-1 and H-1'; 2.34t, J=7.50 (2H), 1.60m (4H), 1.26s (51H), 0.88t (6H); ^{13}C NMR: δ173.97s, 71.81t, 71.46t, 68.93d, 65.46t, 34.23t, 31.95t, 29.71t, 29.63t, 29.50t, 29.38t, 29.29t, 29.17t, 26.11t, 24.97t, 22.70t, 14.12q.

Compound (7) (40mg) in 5ml of 10% methanolic KOH was refluxed for 4 hours. Work up gave 15mg of 1-O-hexadecyl glycerol (8) and 20mg of hexadecanoic acid.

LN02 (13)

Gum (0.03g), $(\alpha)_D^{30}$+1.72° (C,0.58, $CHCl_3$). λ_{max}^{EtOH} 225 nm (log ε 3.99). $C_{20}H_{30}O_3$, found m/z 318 (M^+) and m/z 317.2120 calc. for $C_{20}H_{29}O_3$ 317.2118. For ^1H NMR spectrum see Text.

LN03 (16)

Gum (0.06g), $(\alpha)_D^{30}$-66.7° (C,0.15, $CHCl_3$), $\nu_{max}^{CHCl_3}$ 3601, 907 and 835 cm^{-1}, $C_{20}H_{32}O_2$. Mass spectrum (CI^+): m/z (322) ($M+\dot{N}H_4$) (40%), 305 (M+1) (20), 287 (M-OH) (100), and 269.2314 (correspondence to $C_{20}H_{29}$ ($M-H_2O$, OH), calc. for $C_{20}H_{20}$ m/z 269.2271. For ^1H and ^{13}C NMR spectra see Text.

Mixture of 1-O-hexadecyl glycerol (8) and 1-O-Octadecyl glycerol (9)

Colourless prisms from methanol (0.05g), m.p. 63-64°, $\nu_{max}^{CHCl_3}$ 3550 cm^{-1}. ^1H NMR: δ3.87m (1H), H-2; 3.71m (2H), H-1; 3.50m (4H), H-3 and H-1'; 2.31m (2H), OH; 1.58m (2H), 1.26s (26H), 0.88t (3H); ^{13}C NMR: δ72.53t, 71.90t, 70.49d, 64.33t, 31.95t, 29.71t, 29.62t, 29.41t, 29.38t, 26.11t, 22.70t, 14.12q.

The compound showed as a single spot on TLC but showed two molecular ions in its CI^+ mass spectrum, one at m/z 334.3329 (corresponding to $C_{19}H_{40}O_3 \cdot \dot{N}H_4$, 1-O-hexadecyl glycerol, (8), also known as chimyl alcohol) and the other at m/z 362.3639 (corresponding to $C_{21}H_{44}O_3 \cdot \dot{N}H_4$, 1-O-octadecyl glycerol, (9), also known as batyl alcohol) in almost equal proportions.

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