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A novel aliphatic polyols isolated from the leaves of *Persea gratissimma*

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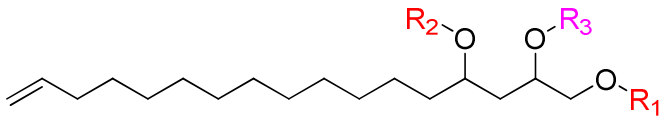
ABSTRACT

*A new long chain polyol-2-isopropoxyheptadec-16-ene-1,4-diol(**1**), 2-isopropoxyheptadec-16-ene-1,4-diyldiacetate (**2**) and Dotriacontane (**3**) were isolated from the leaves of Persea gratissimma. All the isolated compounds (**1-3**) were well characterized by spectral and analytical data.*

Keywords: *Persea gratissimma*, isopropyl ether of aliphatic polyol, Dotriacontane.

INTRODUCTION

The various species of the genus *Persea (Lauraceae)* are widely cultivated for their fruits, popularly known as avocado or alligator pear. **[**1**]** This fruit is reported to have very high protein content, along with other nutrients, such as, riboflavin, thiamine **[**2**]** etc. The aqueous extracts of leaves of *Persea americana* are used for the treatment of cancer **[**3**]** and hypertension. **[**4**]** Extracts of the dried peel and the seeds have antibiotic activity against *Micrococcus pyogenes* and *Sarcina lutea*. **[**5**]** Haslam reported **[**6**]** a number of proanthocyanidins, namely B-1, B-2 and C-1. Kashman *et al*., reported a number of aliphatic triols, such as 16-heptadecene 1,2,4-triol and 16-heptadecyne 1,2,4-triol. **[**7**]** Dotriacontane, nonacosane, β-amyrin, kaempferol and quercetin and a partially characterised steroid and an acylated flavonol isolated from the leaves of *Persea gratissimma*. **[**8**]** We now report in this communication we isolated three novel new longchain polyol compounds ie. 2-isopropoxyheptadec-16-ene-1,4-diol **(1)**, 2-isopropoxyheptadec-16-ene-1,4-diyl diacetate **(2)** and Dotriacontane **(3) (**shown in fig.1) from the leaves of *Persea gratissimma*.



(1) R_1, R_2= H and R_3= isopropyl

(2) R_1, R_2=acetyl and R_3= isopropyl

$H_3C(CH_2)_{30}CH_3$

(3) Dotriacontane

Fig.1. Structures of the synthetic compounds 1-3.

MATERIALS AND METHODS

General methods: Isolation was monitored by thin layer chromatography (TLC) on silica gel plates (60 F254), visualizing with ultraviolet light or iodine spray. ^{1}H NMR and ^{13}C NMR spectra were determined in $CDCl_3$ solution by using 400 and 100MHz spectrometers, respectively. Proton chemical shifts (δ) are relative to tetramethylsilane (TMS, δ = 0.00) as internal standard and expressed in ppm. Spin multiplicities are given as s (singlet), d (doublet), t (triplet) and m (multiplet) as well as b (broad). Coupling constants (*J*) are given in hertz. Infrared spectra were recorded on a FTIR spectrometer. Melting points were determined by using a Buchi melting point B-540 apparatus. MS spectra were obtained on a mass spectrometer.

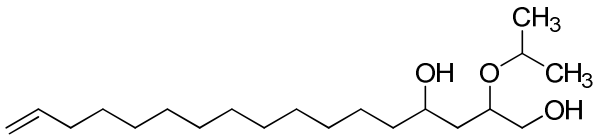
Plant material

Persea gratisima leaves were collected from the Lalbagh gardens at Bangalore, India and dried leaves were used for extraction.

Extraction and isolation

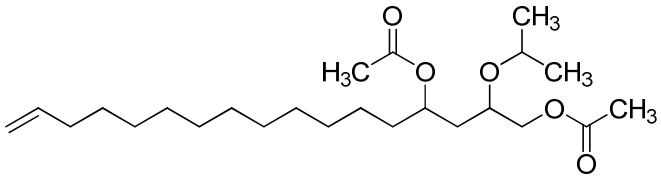
Dried leaves (300 g) were soxhlet extracted with petroleum ether and the extract was concentrated to a viscous mass. A portion of this material (25 g) on column chromatographic separation over Silica gel G using petroleum ether and ethyl acetate mixture to afford the desired products **1-3.** All the isolated compounds were well characterized by spectral (NMR, MS and IR) data.

2-isopropoxyheptadec-16-ene-1,4-diol (1)



A pale white solid, m.p.68ºC; R_f : 0.52 (Silica Gel, Ethyl acetate), did not form an acetonide with dry acetone and anhydrous copper sulphate. Answered 2,4-DNP after reaction with pyridinium chlorochromate. Gave 16-heptadecene-1,2,4-triol on acid (Conc. HCl) hydrolysis. IR bands (nujol): 3300, 1471, 1642, 1371, 1335, 1124, 845 and 720 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$): δ 5.80-5.82 (m, 1H), 4.98 (d, *J* = 4.5 Hz, 2H), 4.00–3.80 (m, 3H), 3.51 (dd, *J* = 3 and 10 Hz, 2H), 2.20-2.10 (m, 2H), 1.75-1.88 (m, 2H), 1.68-1.66 (m, 2H), 1.55 (d, *J* = 3 Hz, 6H), 1.25 (s, 20H); ^{13}C-NMR (100 MHz, $CDCl_3$): 139, 114.7, 77.64, 72.4, 71.7, 66.5, 39, 38, 33.73, 31.8, 29.64, 29.47, 29.2, 29.09, 28.8, 28.7, 28.4, 25.4, 22.6; EIMS m/z: M^+ 329 (9%), 299, 271, 269 (100%), 251, 193, 163, 149, 135, 137 and 133.

2-isopropoxyheptadec-16-ene-1,4-diyl diacetate (2)



Liquid at room temperature, R_f: 0.78 (Silica Gel, Ethyl acetate). IR bands (nujol): 3060, 2920, 2840, 1710, 1650, 1445, 1371, 1355, 1260, 1220, 1045, 1020 and 900 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$): δ 5.80-5.82 (m,1H), 5.10-5.20 (m, 2H), 4.90-4.92 (m, 1H), 4.25 (dd, *J* = 3 and 10 Hz, 2H), 3.85–3.65 (m, 2H), 1.98-2.05 (m, 8H), 1.75-1.88 (m, 2H), 1.55 (d, *J* = 3 Hz, 6H), 1.25 (s, 20H); EIMS m/z (%) M^+ 413(0.3%).

Dotriacontane (3)

$H_3C(CH_2)_{30}CH_3$

Dotriacontane Colorless waxy solid. R_f: 0.89 (Silica gel, petroleum ether [60-80 mesh]. IR bands (nujol): 2910, 2840, 1470, 1460, 1370, 730 and 720 cm^{-1}; EIMS m/z (%) M+. 451(0.05%), 436, 407, 393, 379, 365, 351, 337, 323, 309, 295, 281, 267, 253, 239, 225, 211, 197, 183, 169, 155, 141, 127, 111, 99, 85, 71, 57(100), 43, 29 and 15.

RESULTS AND DISCUSSION

Petroleum ether extract of the dried leaves of *P. gartissimma* on chromatographic separation over silica gel afforded a new compound **1** whose NMR and mass spectrum showed similarity with the earlier reported compound 16-heptadecene–1,2,4 triol, commonly known as avocadene (R_f: 0.63 - silica gel G, ethyl acetate). Its IR absorption indicated hydroxyl and olefinic bonds. The presence of terminal double bond was confirmed from the signals in ^{1}H-NMR and ^{13}C-NMR. The ^{1}H-NMR showed additional 1H multiplet at δ 3.9 and a six-proton doublet at δ 1.5 indicating the presence of an isopropyl ether group. This conjuncture was supported from its IR spectrum, which showed a characteristic strong absorption at 1335 and 1371 cm^{-1} for gem dimethyl group.

The compound-**1** gave negative result with benzidine/periodate unlike avocadene showing the absence of 1,2-diol, and gave positive result for polyols (alkaline potassium permanganate). Unlike avocadene, the compound did not form either the acetonide or the benzylidene derivatives, indicating the absence of a 1,2 and a 1,3–diol systems and a substitution at the hydroxyl at carbon-2. The carbinol protons resonated at δ 3.44 (m, 1H), 3.61 (dd, 2H), 3.90 (m, 1H) and 3.91(m, 1H). While, in the acetate derivative (**2**) the carbinol protons resonated at δ 3.85 (m, 1H), 4.01 (m, 1H), 4.25 (dd, 2H) and 4.85 (m, 1H). The down field shift of the H-1 and H-4 protons in the acetate, indicate the substitution of the hydroxyl at carbon-2. Acid hydrolysis of compound-**1** with concentrated hydrochloric acid yielded avocadene, confirming that the compound-**1** is an isopropyl derivative of avocadene. Its Mass spectrum gave a M^+ at m/z 328 along with a prominent $[M\text{-}C_3H_7O]^+$ peak at m/z 269. The rest of the peaks were similar to the Mass spectrum of avocadene. From the above observations and its ^{13}C-NMR data the compound-1 and 2 were deduced to be 2-isopropoxyheptadec-16-ene-1,4-diol (**1**) and 2-isopropoxyheptadec-16-ene-1,4-diyl diacetate (**2**). Dotriacontane is an alkane with 32 carbons was isolated and compared with reported literature procedure. **[**8-9**]**

CONCLUSION

In conclusion, A new longchain polyol 2-isopropoxyheptadec-16-ene-1,4-diol (**1**), 2-isopropoxyheptadec-16-ene-1,4-diyl diacetate (**2**) and Dotriacontane (**3**) were isolated from the leaves of *Persea gratissimma*. All the isolated compounds (**1**-**3**) were well characterized by spectral (NMR, MS and IR) data.

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